Fig. 1

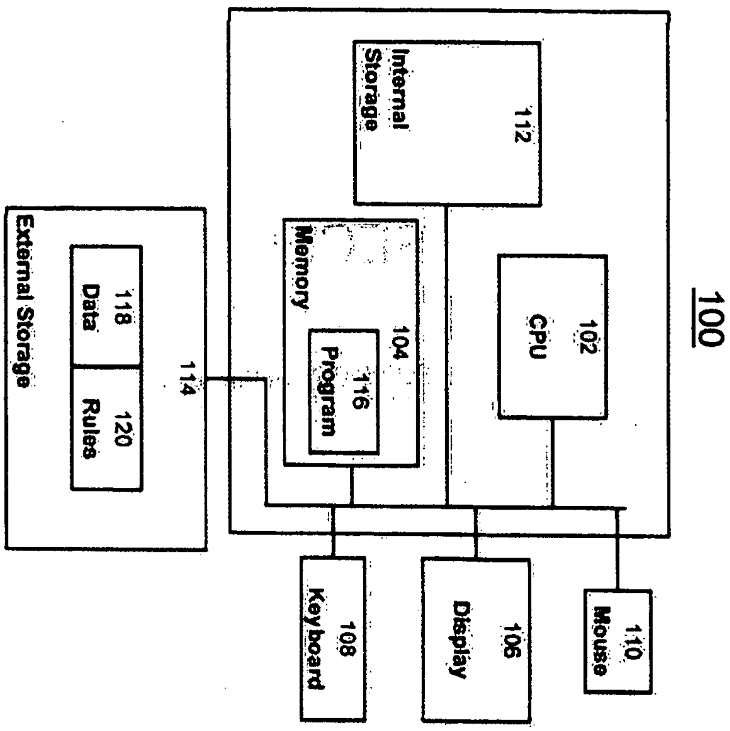
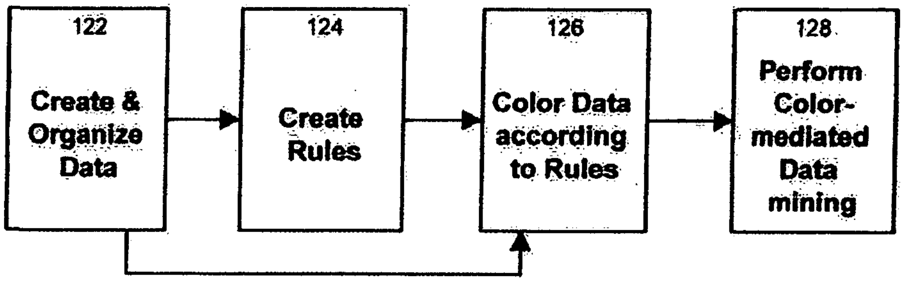
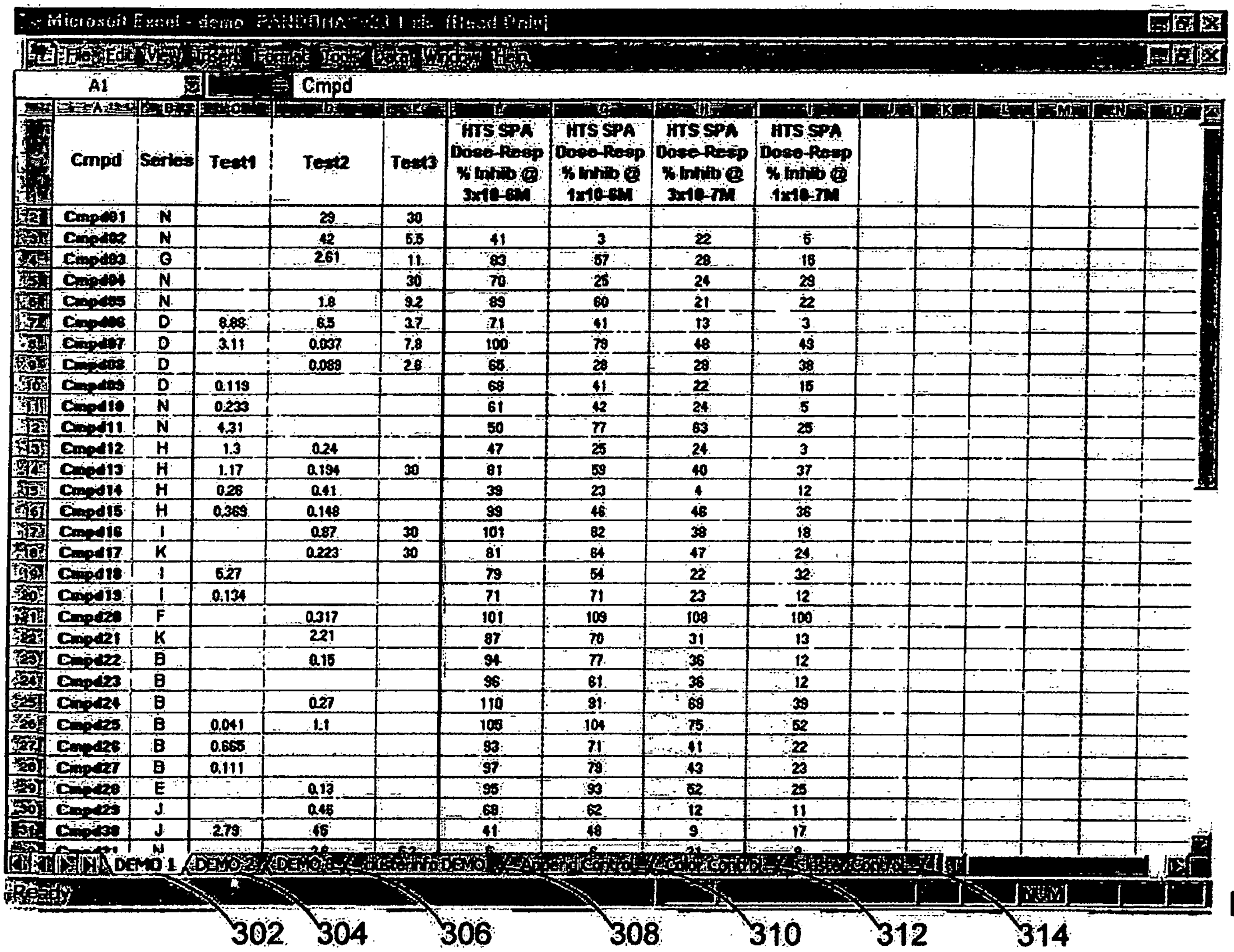

100
102
CPU
112
Internal Storage
104
Memory
116
Program
114
External Storage
118
Data
120
Rules
110
Mouse
106
Display
108
Keyboard

Fig. 2

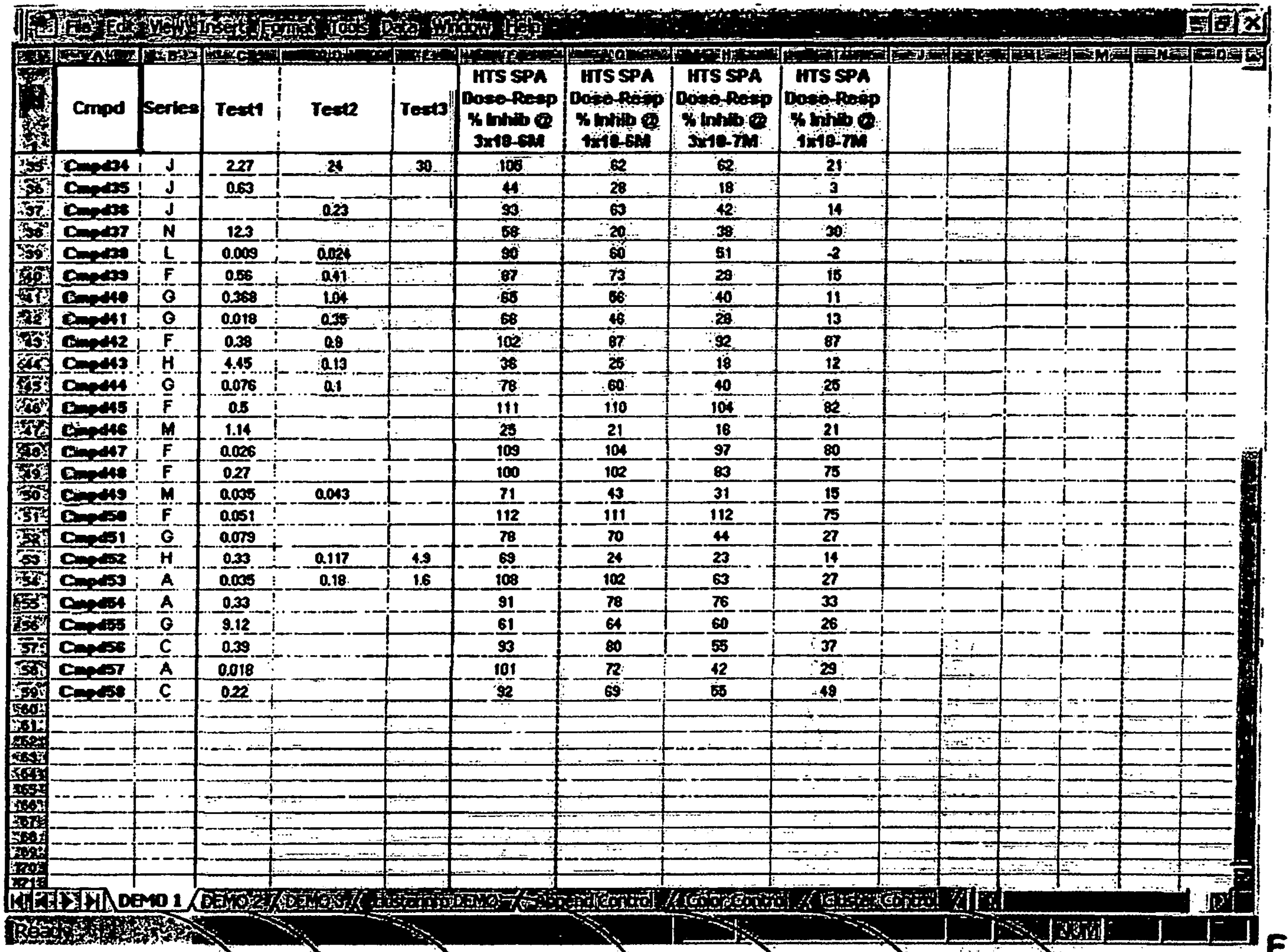

122
Create & Organize Data
124
Create Rules
126
Color Data according to Rules
128
Perform Color-mediated Data mining

300



Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
Cmpd01	N		29	30				
Cmpd02	N		42	5.5	41	3	22	6
Cmpd03	G		2.61	11	83	57	28	18
Cmpd04	N			30	70	25	24	29
Cmpd05	N		1.8	9.2	89	60	21	22
Cmpd06	D	8.88	8.5	3.7	71	41	13	3
Cmpd07	D	3.11	0.037	7.8	100	79	48	43
Cmpd08	D		0.089	2.6	65	28	29	38
Cmpd09	D	0.119			68	41	22	15
Cmpd10	N	0.233			61	42	24	5
Cmpd11	N	4.31			50	77	63	25
Cmpd12	H	1.3	0.24		47	25	24	3
Cmpd13	H	1.17	0.194	30	81	59	40	37
Cmpd14	H	0.26	0.41		39	23	4	12
Cmpd15	H	0.369	0.148		99	46	48	36
Cmpd16	I		0.87	30	101	82	38	18
Cmpd17	K		0.223	30	81	64	47	24
Cmpd18	I	5.27			79	54	22	32
Cmpd19	I	0.134			71	71	23	12
Cmpd20	F		0.317		101	109	108	100
Cmpd21	K		2.21		87	70	31	13
Cmpd22	B		0.15		94	77	36	12
Cmpd23	B				96	61	36	12
Cmpd24	B		0.27		110	91	69	39
Cmpd25	B	0.041	1.1		106	104	75	52
Cmpd26	B	0.665			93	71	41	22
Cmpd27	B	0.111			97	79	43	23
Cmpd28	E		0.13		95	93	52	25
Cmpd29	J		0.46		68	62	12	11
Cmpd30	J	2.79	46		41	48	9	17

Fig. 3A



	Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
35	Cmpd34	J	2.27	24	30	106	62	62	21
36	Cmpd35	J	0.63			44	28	18	3
37	Cmpd36	J		0.23		93	63	42	14
38	Cmpd37	N	12.3			58	20	38	30
39	Cmpd38	L	0.009	0.024		90	60	51	-2
40	Cmpd39	F	0.56	0.41		87	73	29	15
41	Cmpd40	G	0.368	1.04		65	66	40	11
42	Cmpd41	G	0.018	0.35		68	46	28	13
43	Cmpd42	F	0.38	0.9		102	87	92	87
44	Cmpd43	H	4.45	0.13		38	25	18	12
45	Cmpd44	G	0.076	0.1		78	60	40	25
46	Cmpd45	F	0.5			111	110	104	82
47	Cmpd46	M	1.14			25	21	16	21
48	Cmpd47	F	0.026			109	104	97	80
49	Cmpd48	F	0.27			100	102	83	75
50	Cmpd49	M	0.035	0.043		71	43	31	15
51	Cmpd50	F	0.051			112	111	112	75
52	Cmpd51	G	0.079			78	70	44	27
53	Cmpd52	H	0.33	0.117	4.9	69	24	23	14
54	Cmpd53	A	0.035	0.18	1.6	108	102	63	27
55	Cmpd54	A	0.33			91	78	76	33
56	Cmpd55	G	9.12			61	64	60	26
57	Cmpd56	C	0.39			93	80	55	37
58	Cmpd57	A	0.018			101	72	42	29
59	Cmpd58	C	0.22			92	69	65	49

Fig. 3B

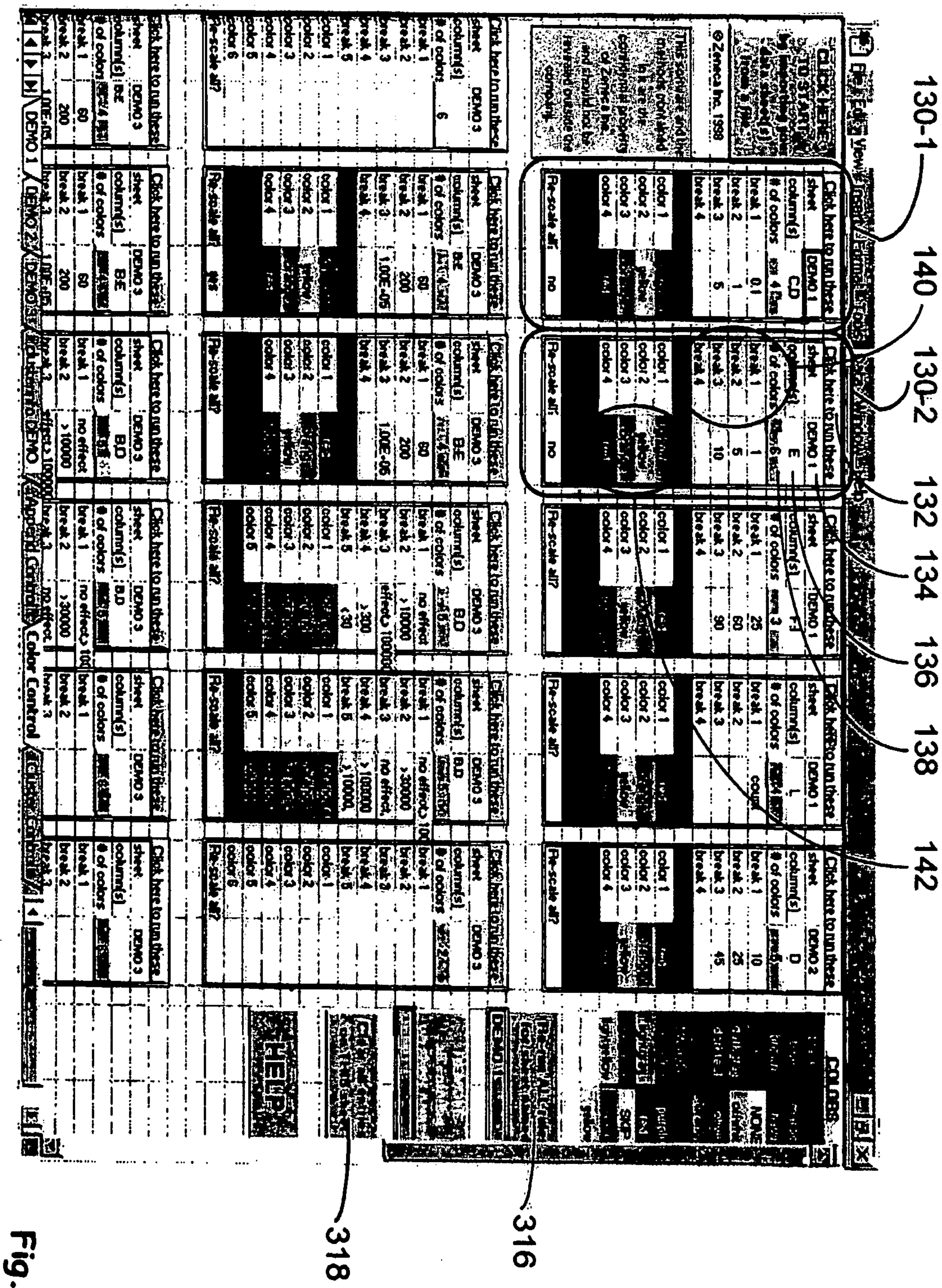
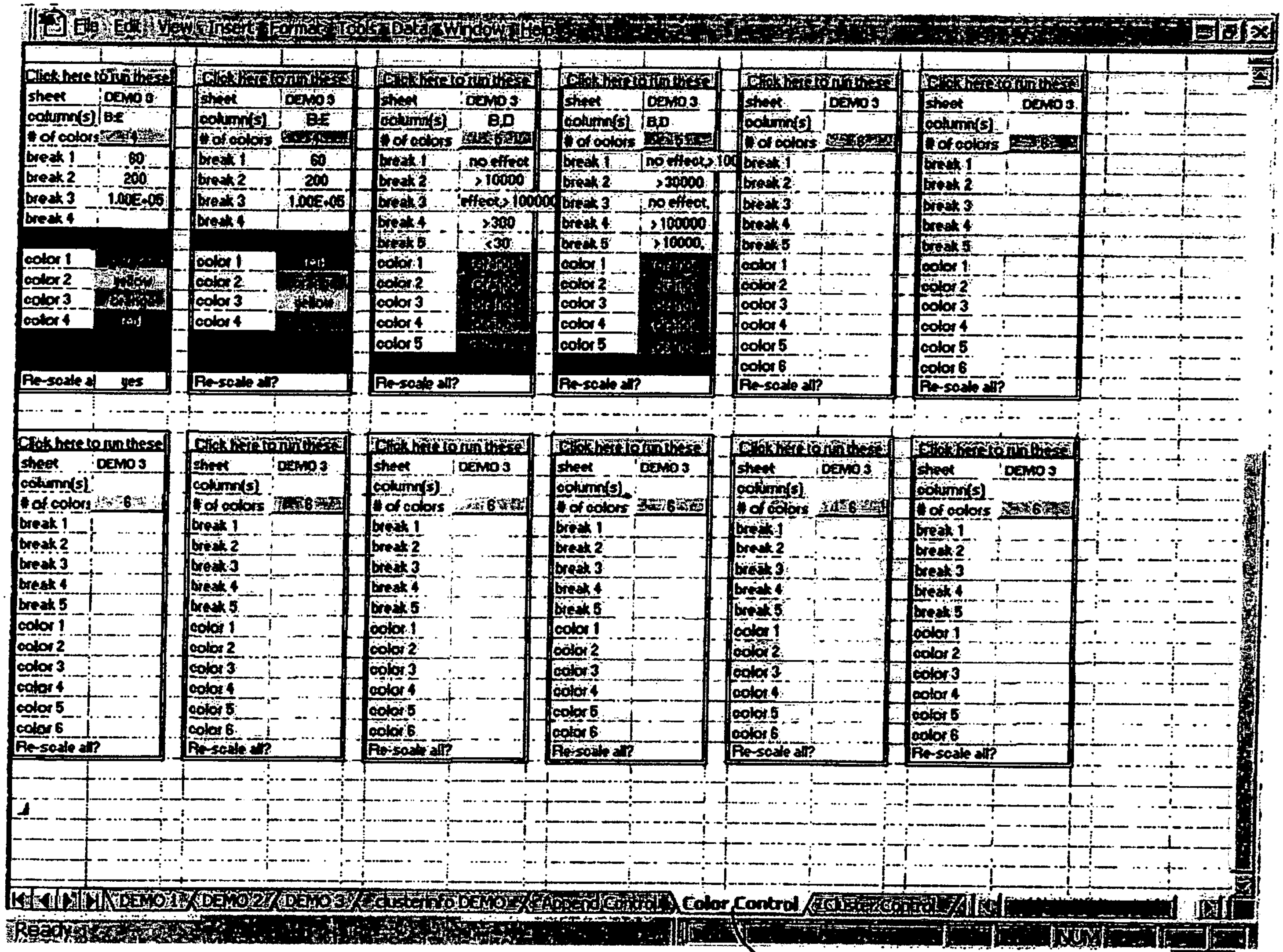


Fig. 4A



Click here to run these	
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column(s)	B:E
# of colors	4
break 1	60
break 2	200
break 3	1.00E+05
break 4	
color 1	[illegible]
color 2	yellow
color 3	orange
color 4	red
Re-scale al	yes

Click here to run these	
sheet	DEMO 3
column(s)	B:E
# of colors	[illegible]
break 1	60
break 2	200
break 3	1.00E+05
break 4	
color 1	red
color 2	[illegible]
color 3	yellow
color 4	[illegible]
Re-scale all?	

Click here to run these	
sheet	DEMO 3
column(s)	B,D
# of colors	[illegible]
break 1	no effect
break 2	>10000
break 3	effect,> 100000
break 4	>300
break 5	<30
color 1	[illegible]
color 2	[illegible]
color 3	[illegible]
color 4	[illegible]
color 5	[illegible]
Re-scale all?	

Click here to run these	
sheet	DEMO 3
column(s)	B,D
# of colors	5
break 1	no effect,> 100
break 2	>30000
break 3	no effect,
break 4	>100000
break 5	>10000,
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color 2	[illegible]
color 3	[illegible]
color 4	[illegible]
color 5	[illegible]
Re-scale all?	

Click here to run these	
sheet	DEMO 3
column(s)	
# of colors	6
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break 2	
break 3	
break 4	
break 5	
color 1	
color 2	
color 3	
color 4	
color 5	
color 6	
Re-scale all?	

Click here to run these	
sheet	DEMO 3
column(s)	
# of colors	6
break 1	
break 2	
break 3	
break 4	
break 5	
color 1	
color 2	
color 3	
color 4	
color 5	
color 6	
Re-scale all?	

Click here to run these	
sheet	DEMO 3
column(s)	
# of colors	6
break 1	
break 2	
break 3	
break 4	
break 5	
color 1	
color 2	
color 3	
color 4	
color 5	
color 6	
Re-scale all?	

Click here to run these	
sheet	DEMO 3
column(s)	
# of colors	6
break 1	
break 2	
break 3	
break 4	
break 5	
color 1	
color 2	
color 3	
color 4	
color 5	
color 6	
Re-scale all?	

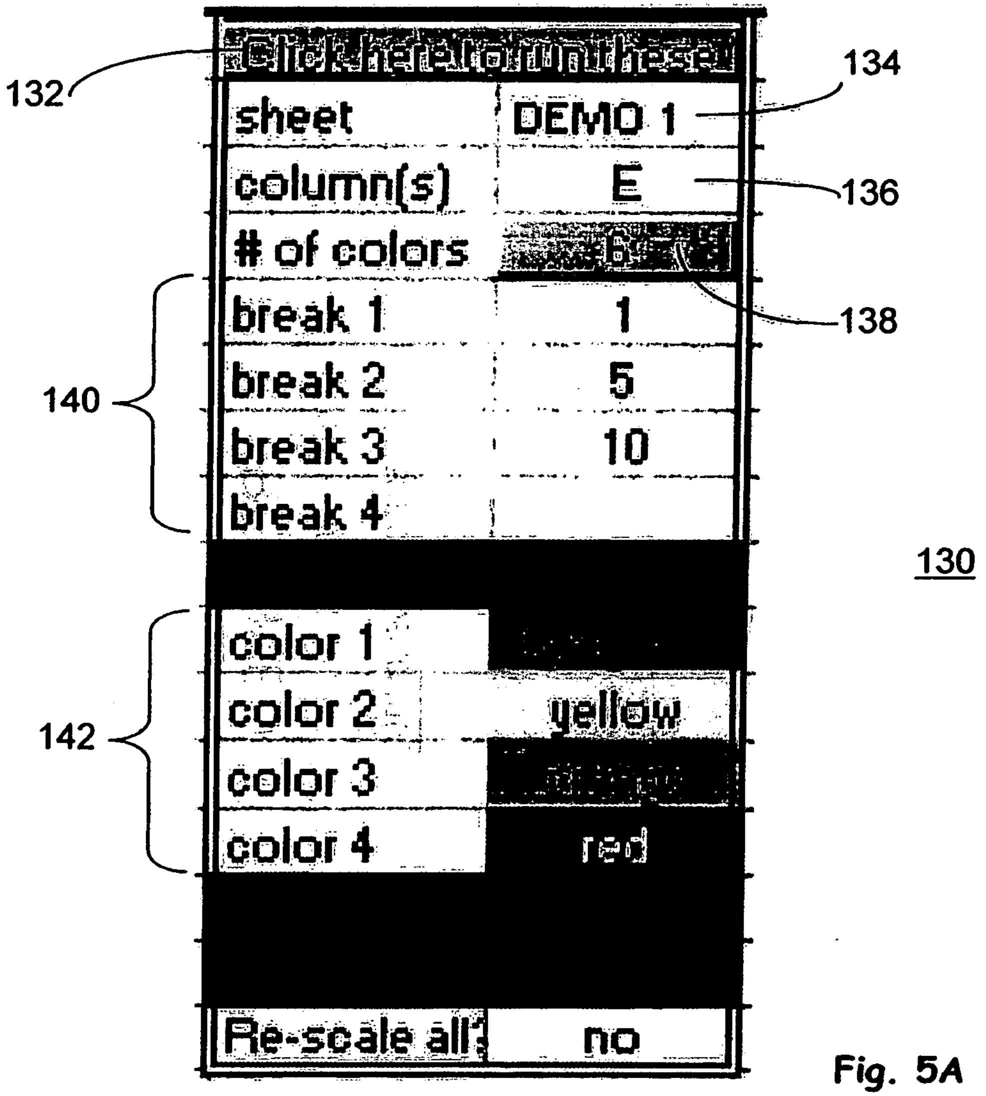
Click here to run these	
sheet	DEMO 3
column(s)	
# of colors	6
break 1	
break 2	
break 3	
break 4	
break 5	
color 1	
color 2	
color 3	
color 4	
color 5	
color 6	
Re-scale all?	

Click here to run these	
sheet	DEMO 3
column(s)	
# of colors	6
break 1	
break 2	
break 3	
break 4	
break 5	
color 1	
color 2	
color 3	
color 4	
color 5	
color 6	
Re-scale all?	

Click here to run these	
sheet	DEMO 3
column(s)	
# of colors	6
break 1	
break 2	
break 3	
break 4	
break 5	
color 1	
color 2	
color 3	
color 4	
color 5	
color 6	
Re-scale all?	

Click here to run these	
sheet	DEMO 3
column(s)	
# of colors	6
break 1	
break 2	
break 3	
break 4	
break 5	
color 1	
color 2	
color 3	
color 4	
color 5	
color 6	
Re-scale all?	

Fig. 4B



Click here to run these

sheet	DEMO 1
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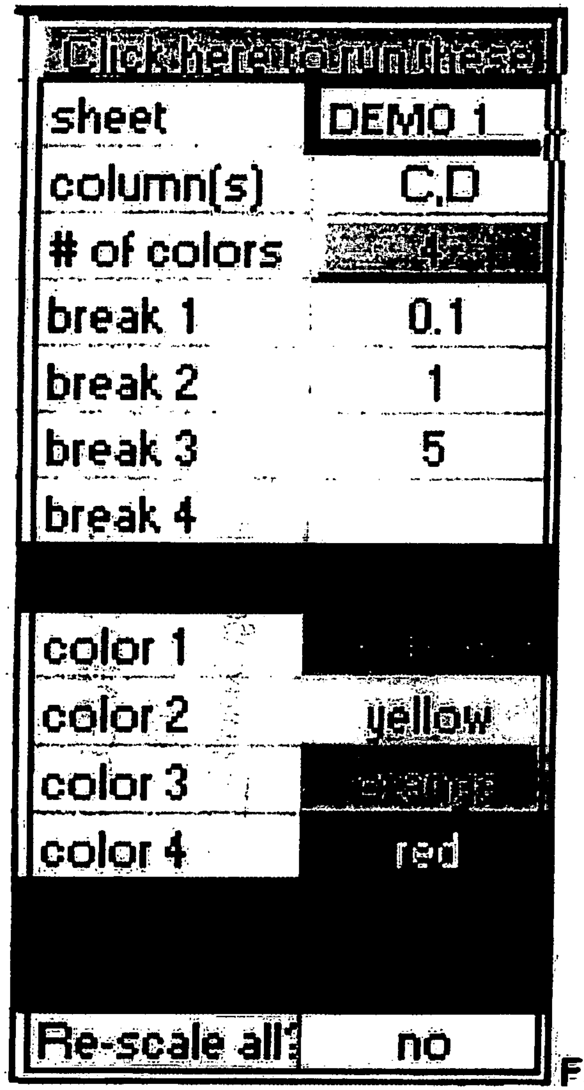
break 2	5
break 3	10
break 4	
color 1	[illegible]
color 2	yellow
color 3	[illegible]
color 4	red
Re-scale all?	no

Fig. 5A



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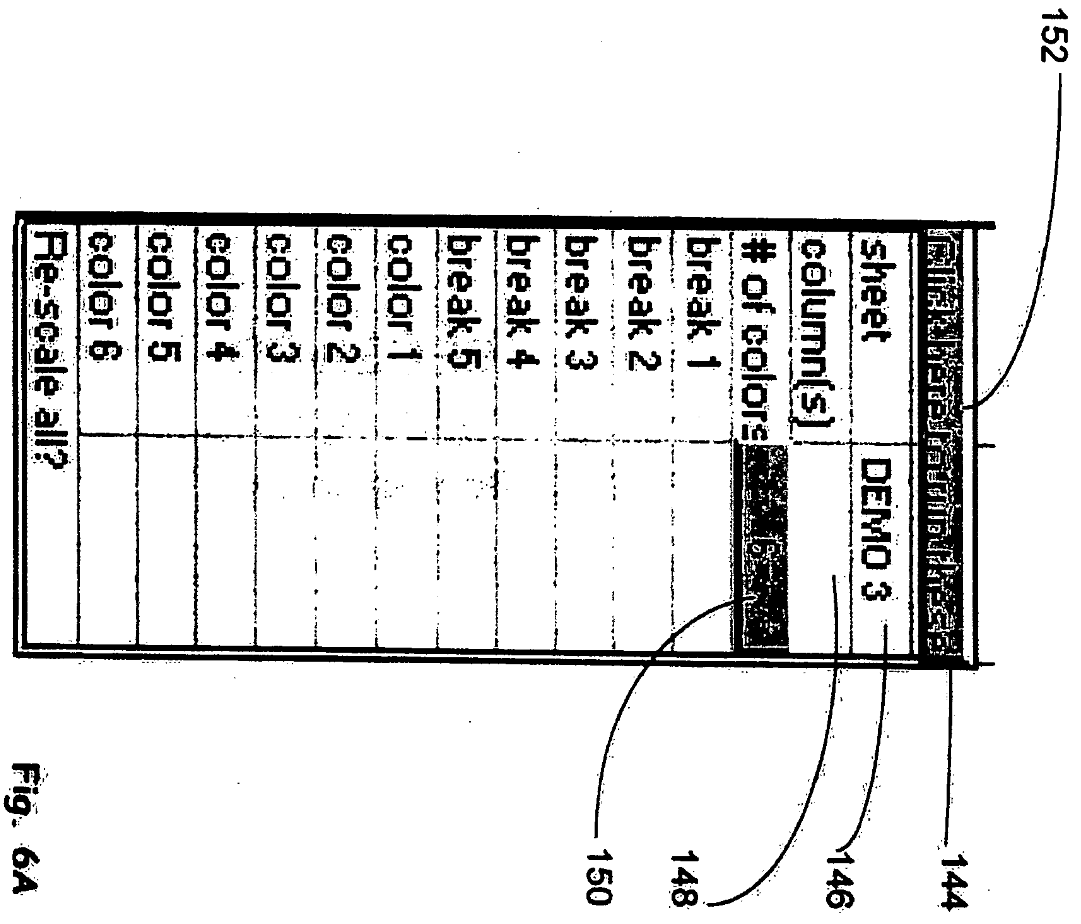
break 3	5
break 4	
color 1	[illegible]
color 2	yellow
color 3	orange
color 4	red
Re-scale all?	no

Fig. 5B



sheet	DEMO 3
column(s)	
# of colors	
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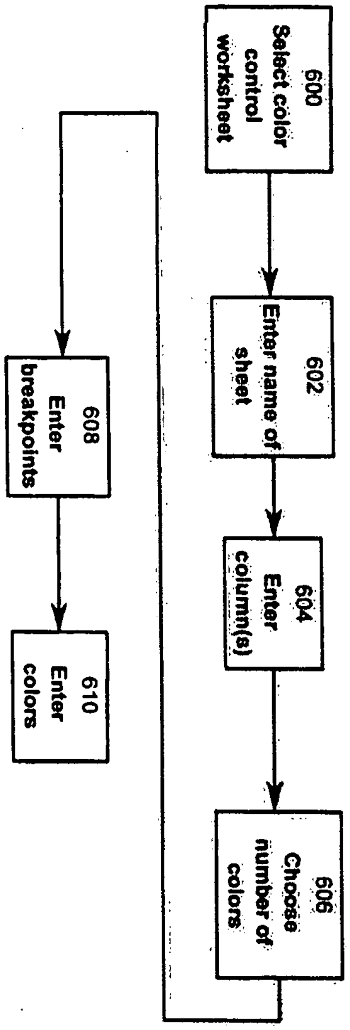
break 2	
break 3	
break 4	
break 5	
color 1	
color 2	
color 3	
color 4	
color 5	
color 6	
Re-scale all?	

Fig. 6A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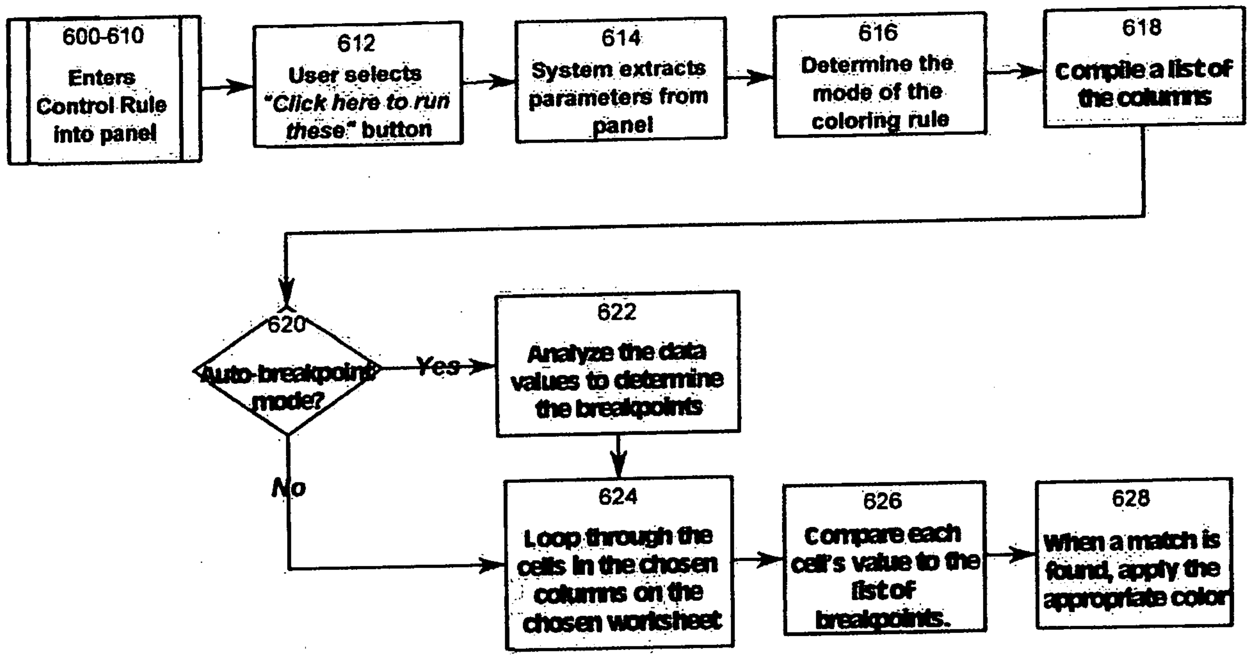
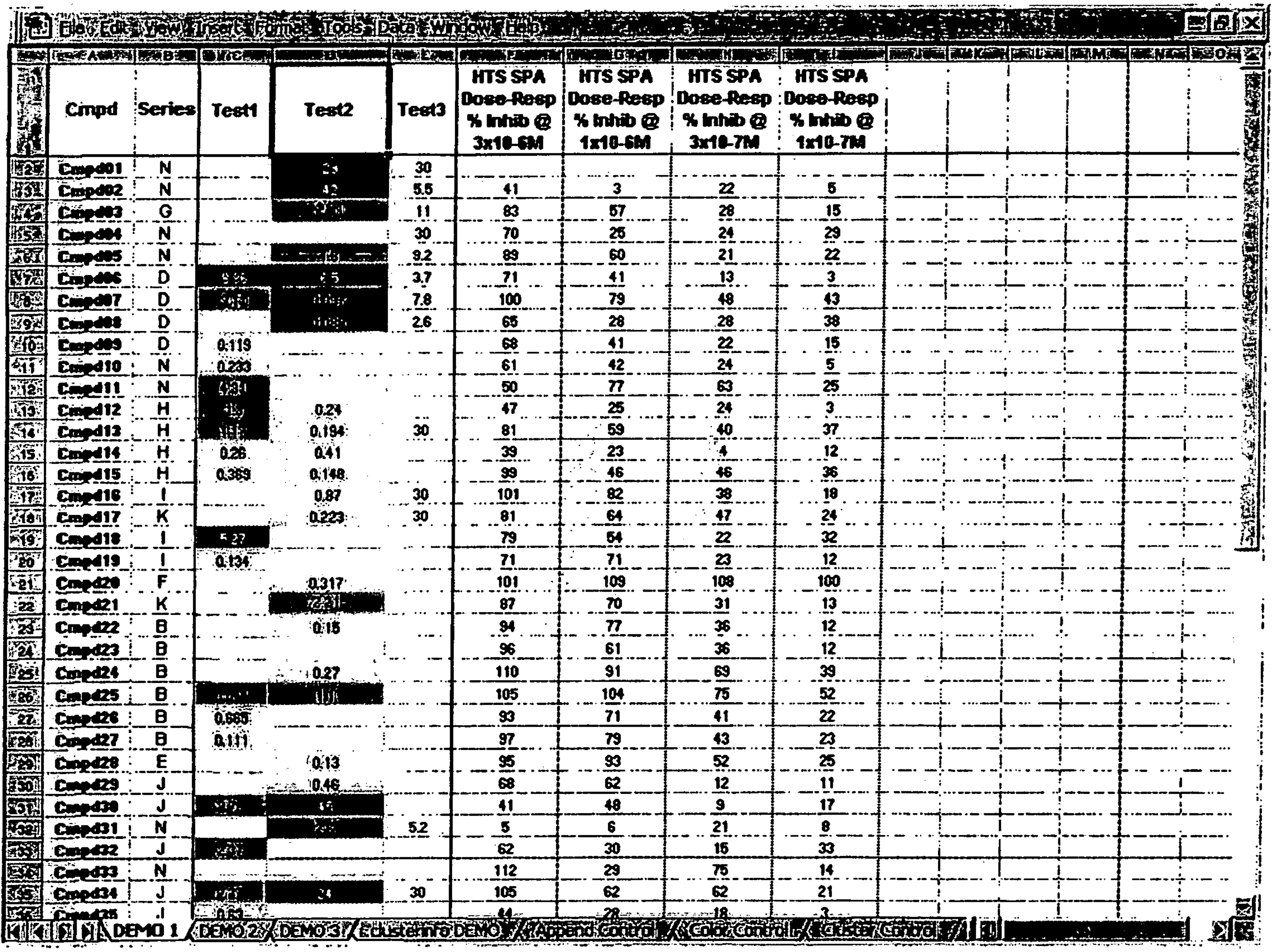
Select color control worksheet
602
Enter name of sheet
604
Enter column(s)
606
Choose number of colors
608
Enter breakpoints
610
Enter colors

Fig. 6B

Fig. 6C

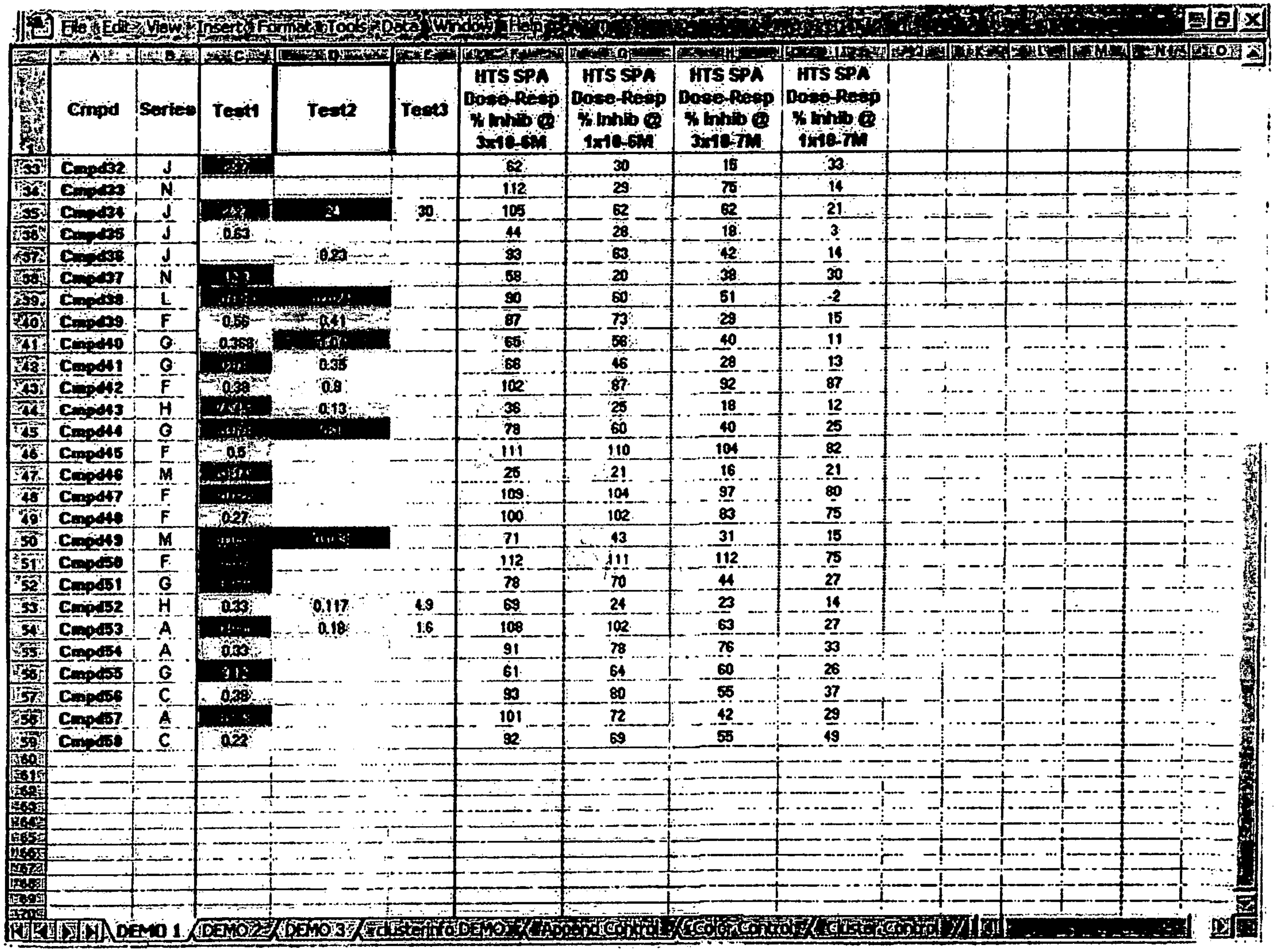

600-610
Enters Control Rule into panel
612
User selects *"Click here to run these"* button
614
System extracts parameters from panel
616
Determine the mode of the coloring rule
618
Compile a list of the columns
620
Auto-breakpoint mode?
Yes
No
622
Analyze the data values to determine the breakpoints
624
Loop through the cells in the chosen columns on the chosen worksheet
626
Compare each cell's value to the list of breakpoints.
628
When a match is found, apply the appropriate color

USSN 10/048,022
LERMAN
Sheet 12 of 64



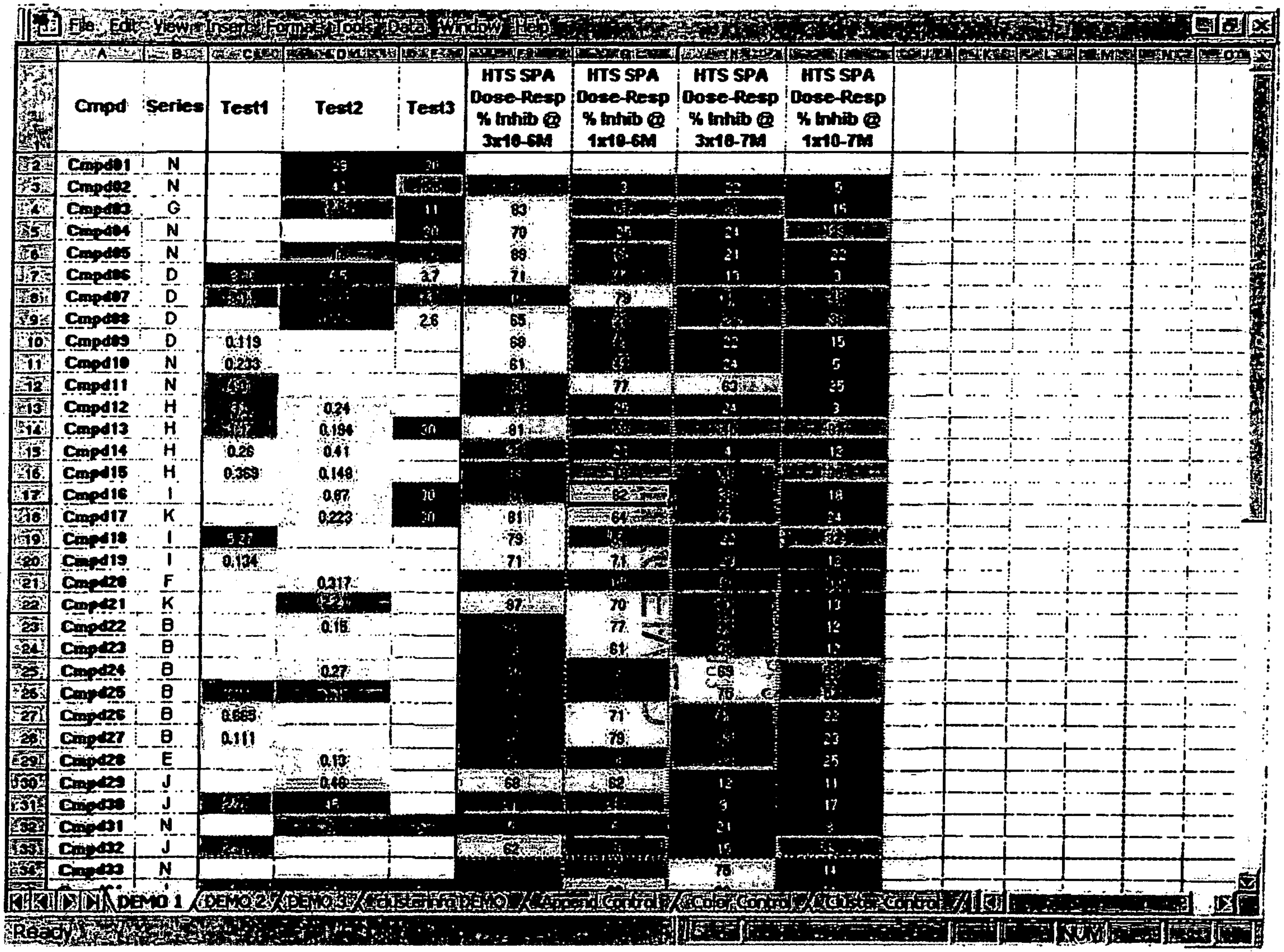
Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
Cmpd01	N		[illegible]	30				
Cmpd02	N		42	5.6	41	3	22	5
Cmpd03	G		[illegible]	11	83	57	28	15
Cmpd04	N			30	70	25	24	29
Cmpd05	N		[illegible]	9.2	89	60	21	22
Cmpd06	D	9.96	6.5	3.7	71	41	13	3
Cmpd07	D	[illegible]	[illegible]	7.8	100	79	48	43
Cmpd08	D		[illegible]	2.6	65	28	28	38
Cmpd09	D	0.119			68	41	22	15
Cmpd10	N	0.233			61	42	24	5
Cmpd11	N	[illegible]			50	77	63	25
Cmpd12	H	[illegible]	0.24		47	25	24	3
Cmpd13	H	[illegible]	0.194	30	81	59	40	37
Cmpd14	H	0.26	0.41		39	23	4	12
Cmpd15	H	0.369	0.148		99	46	46	36
Cmpd16	I		0.87	30	101	82	38	18
Cmpd17	K		0.223	30	81	64	47	24
Cmpd18	I	5.27			79	54	22	32
Cmpd19	I	0.134			71	71	23	12
Cmpd20	F		0.317		101	109	108	100
Cmpd21	K		2.21		87	70	31	13
Cmpd22	B		0.15		94	77	36	12
Cmpd23	B				96	61	36	12
Cmpd24	B		0.27		110	91	69	39
Cmpd25	B	[illegible]	[illegible]		105	104	75	52
Cmpd26	B	0.065			93	71	41	22
Cmpd27	B	0.111			97	79	43	23
Cmpd28	E		0.13		95	93	52	25
Cmpd29	J		0.46		68	62	12	11
Cmpd30	J	[illegible]	[illegible]		41	48	9	17
Cmpd31	N		[illegible]	5.2	5	6	21	8
Cmpd32	J	[illegible]			62	30	15	33
Cmpd33	N				112	29	75	14
Cmpd34	J	[illegible]	34	30	105	62	62	21
Cmpd35	J	[illegible]			44	28	18	3

Fig. 7A



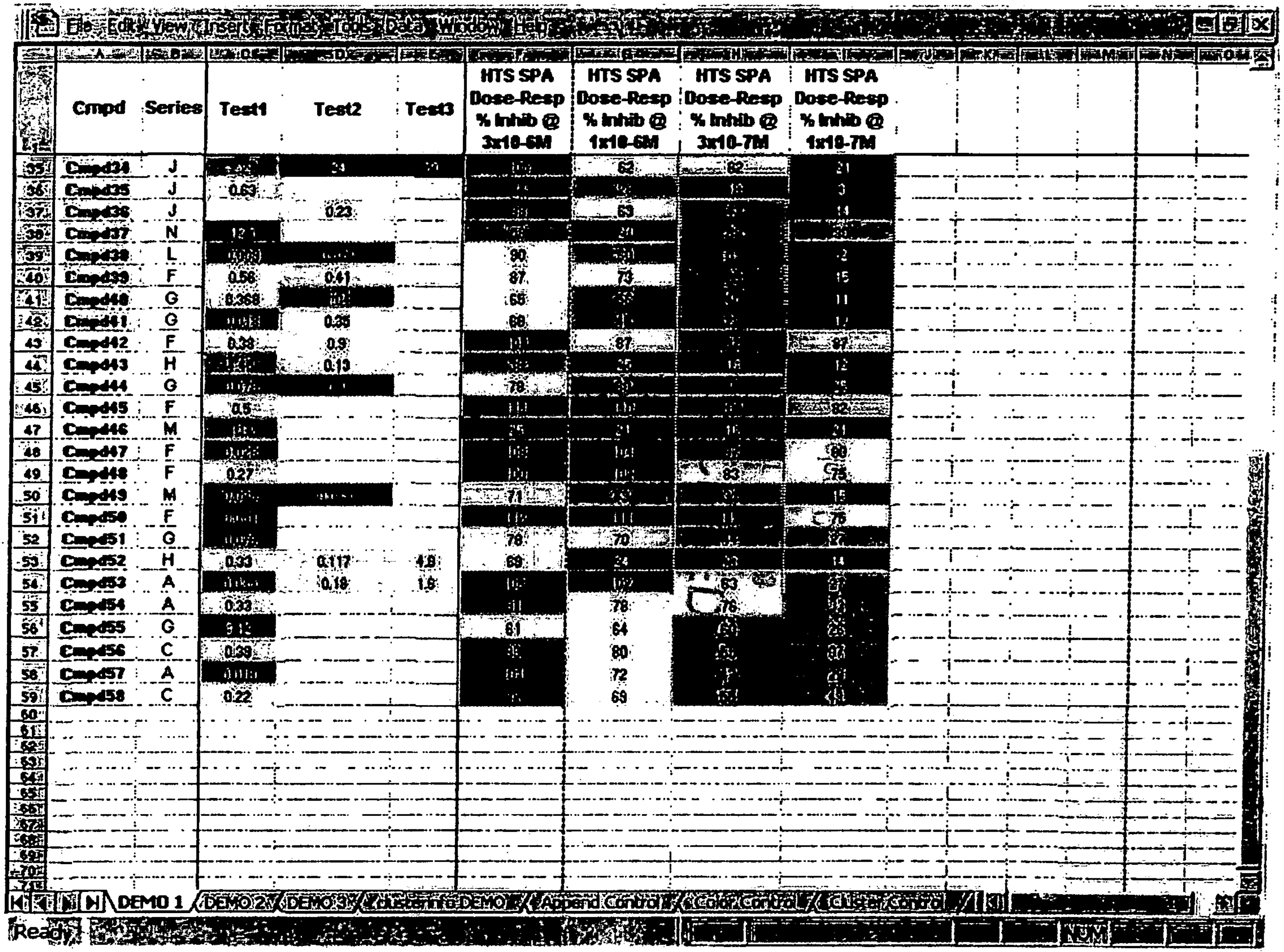
	Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
33	Cmpd32	J	[illegible]			62	30	15	33
34	Cmpd33	N				112	29	75	14
35	Cmpd34	J	[illegible]	24	30	105	62	62	21
36	Cmpd35	J	0.63			44	28	18	3
37	Cmpd36	J		0.23		93	63	42	14
38	Cmpd37	N	[illegible]			58	20	38	30
39	Cmpd38	L	[illegible]	[illegible]		90	60	51	-2
40	Cmpd39	F	0.56	0.41		87	73	29	15
41	Cmpd40	G	0.363	[illegible]		65	56	40	11
42	Cmpd41	G	[illegible]	0.35		68	46	28	13
43	Cmpd42	F	0.38	0.8		102	87	92	87
44	Cmpd43	H	[illegible]	0.13		36	25	18	12
45	Cmpd44	G	[illegible]	[illegible]		78	60	40	25
46	Cmpd45	F	0.5			111	110	104	82
47	Cmpd46	M	[illegible]			25	21	16	21
48	Cmpd47	F	[illegible]			109	104	97	80
49	Cmpd48	F	0.27			100	102	83	75
50	Cmpd49	M	[illegible]	[illegible]		71	43	31	15
51	Cmpd50	F	[illegible]			112	111	112	75
52	Cmpd51	G	[illegible]			78	70	44	27
53	Cmpd52	H	0.33	0.117	4.9	69	24	23	14
54	Cmpd53	A	[illegible]	0.18	1.6	108	102	63	27
55	Cmpd54	A	0.33			91	78	76	33
56	Cmpd55	G	[illegible]			61	64	60	26
57	Cmpd56	C	0.39			93	80	55	37
58	Cmpd57	A	[illegible]			101	72	42	29
59	Cmpd58	C	0.22			92	69	55	49

Fig. 7B



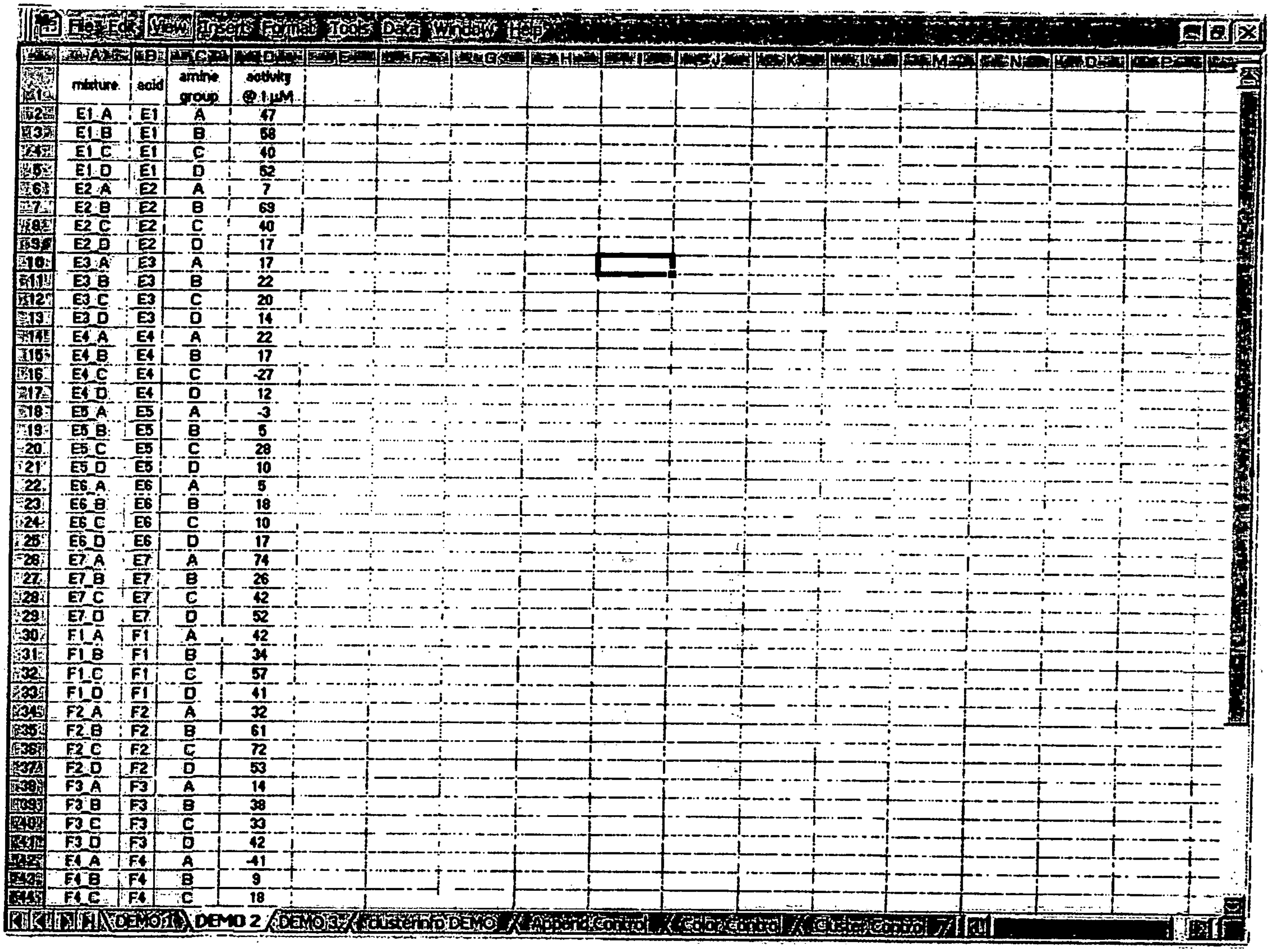
Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
Cmpd01	N		39	30				
Cmpd02	N		42	[illegible]	[illegible]	3	22	5
Cmpd03	G		[illegible]	11	83	[illegible]	[illegible]	15
Cmpd04	N			30	70	25	24	[illegible]
Cmpd05	N		[illegible]	[illegible]	88	[illegible]	21	22
Cmpd06	D	[illegible]	4.5	3.7	71	[illegible]	15	3
Cmpd07	D	[illegible]	[illegible]	[illegible]	[illegible]	79	[illegible]	[illegible]
Cmpd08	D		[illegible]	2.6	65	[illegible]	[illegible]	[illegible]
Cmpd09	D	0.119			68	[illegible]	22	15
Cmpd10	N	0.233			61	[illegible]	24	5
Cmpd11	N	[illegible]			[illegible]	77	63	25
Cmpd12	H	[illegible]	0.24		[illegible]	25	24	3
Cmpd13	H	[illegible]	0.194	30	81	[illegible]	[illegible]	[illegible]
Cmpd14	H	0.26	0.41		[illegible]	21	4	12
Cmpd15	H	0.369	0.149		[illegible]	[illegible]	[illegible]	[illegible]
Cmpd16	I		0.07	30	[illegible]	82	[illegible]	18
Cmpd17	K		0.223	30	81	64	[illegible]	24
Cmpd18	I	5.27			79	[illegible]	22	[illegible]
Cmpd19	I	0.134			71	71	[illegible]	12
Cmpd20	F		0.317		[illegible]	[illegible]	[illegible]	[illegible]
Cmpd21	K		[illegible]		97	70	[illegible]	13
Cmpd22	B		0.15		[illegible]	77	[illegible]	12
Cmpd23	B				[illegible]	61	[illegible]	12
Cmpd24	B		0.27		[illegible]	[illegible]	69	[illegible]
Cmpd25	B	[illegible]	[illegible]		[illegible]	[illegible]	76	[illegible]
Cmpd26	B	0.665			[illegible]	71	[illegible]	22
Cmpd27	B	0.111			[illegible]	79	[illegible]	23
Cmpd28	E		0.13		[illegible]	[illegible]	[illegible]	25
Cmpd29	J		0.46		68	62	12	11
Cmpd30	J	[illegible]	15		[illegible]	[illegible]	9	17
Cmpd31	N		[illegible]	[illegible]	[illegible]	[illegible]	21	3
Cmpd32	J	[illegible]			62	[illegible]	15	[illegible]
Cmpd33	N				[illegible]	[illegible]	75	14

Fig. 8A



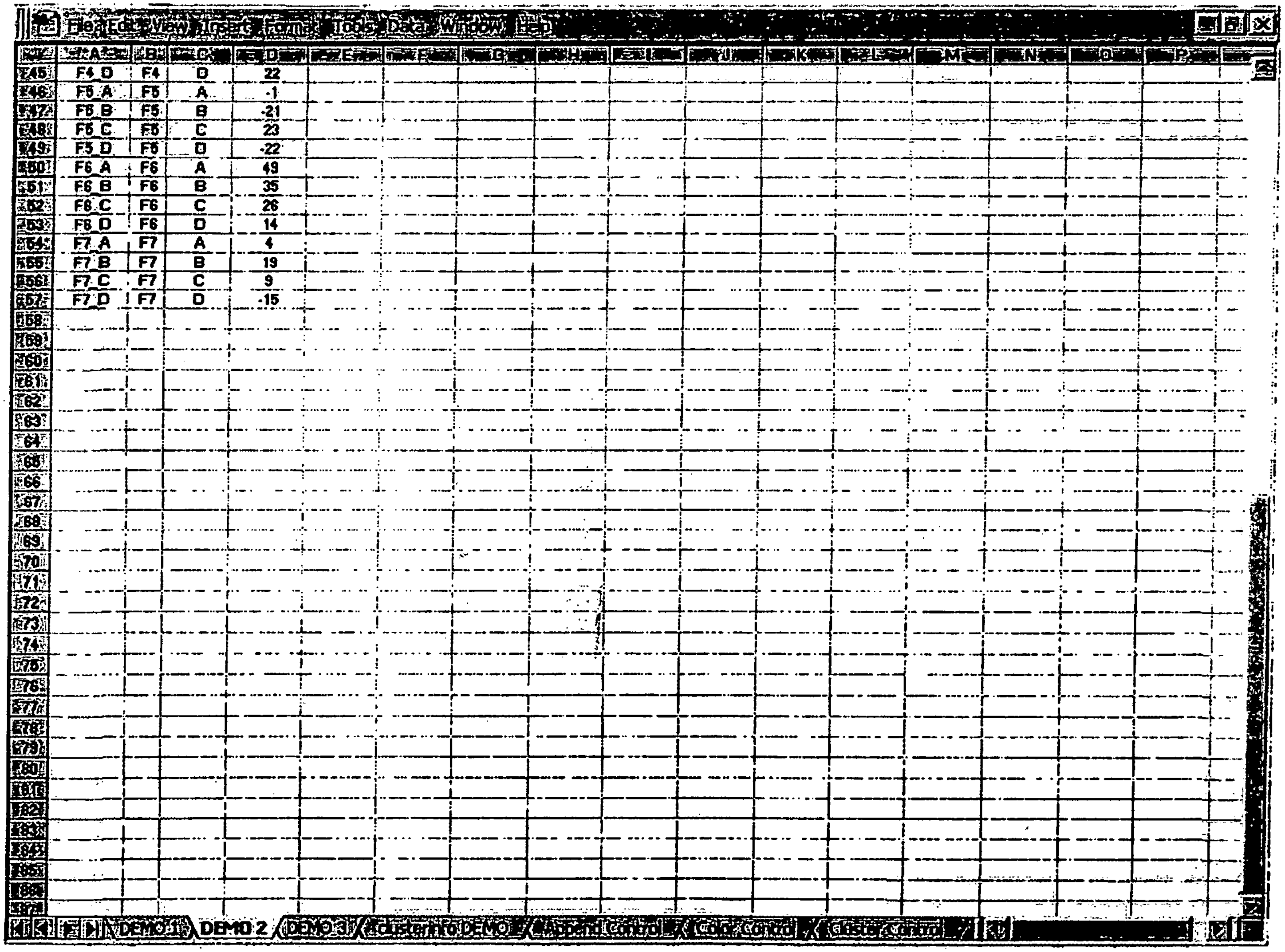
	Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
35	Cmpd34	J	[illegible]	24	[illegible]	[illegible]	62	82	21
36	Cmpd35	J	0.63			[illegible]	[illegible]	18	3
37	Cmpd36	J		0.23		[illegible]	69	[illegible]	14
38	Cmpd37	N	[illegible]			[illegible]	20	[illegible]	[illegible]
39	Cmpd38	L	[illegible]	[illegible]		90	[illegible]	[illegible]	-2
40	Cmpd39	F	0.56	0.41		87	73	[illegible]	15
41	Cmpd40	G	0.368	[illegible]		68	[illegible]	[illegible]	11
42	Cmpd41	G	[illegible]	0.35		69	[illegible]	[illegible]	12
43	Cmpd42	F	0.38	0.9		[illegible]	87	[illegible]	87
44	Cmpd43	H	[illegible]	0.13		[illegible]	25	18	12
45	Cmpd44	G	[illegible]	[illegible]		78	[illegible]	[illegible]	25
46	Cmpd45	F	0.5			[illegible]	[illegible]	[illegible]	82
47	Cmpd46	M	[illegible]			25	21	15	21
48	Cmpd47	F	[illegible]			[illegible]	[illegible]	[illegible]	80
49	Cmpd48	F	0.27			[illegible]	[illegible]	83	75
50	Cmpd49	M	[illegible]	[illegible]		71	[illegible]	[illegible]	15
51	Cmpd50	F	[illegible]			[illegible]	111	11	75
52	Cmpd51	G	[illegible]			78	70	[illegible]	[illegible]
53	Cmpd52	H	0.33	0.117	4.9	69	24	[illegible]	14
54	Cmpd53	A	[illegible]	0.18	1.6	[illegible]	102	83	[illegible]
55	Cmpd54	A	0.33			[illegible]	78	76	[illegible]
56	Cmpd55	G	[illegible]			61	64	[illegible]	[illegible]
57	Cmpd56	C	0.39			[illegible]	80	[illegible]	[illegible]
58	Cmpd57	A	[illegible]			[illegible]	72	[illegible]	[illegible]
59	Cmpd58	C	0.22			[illegible]	69	[illegible]	[illegible]

Fig. 8B



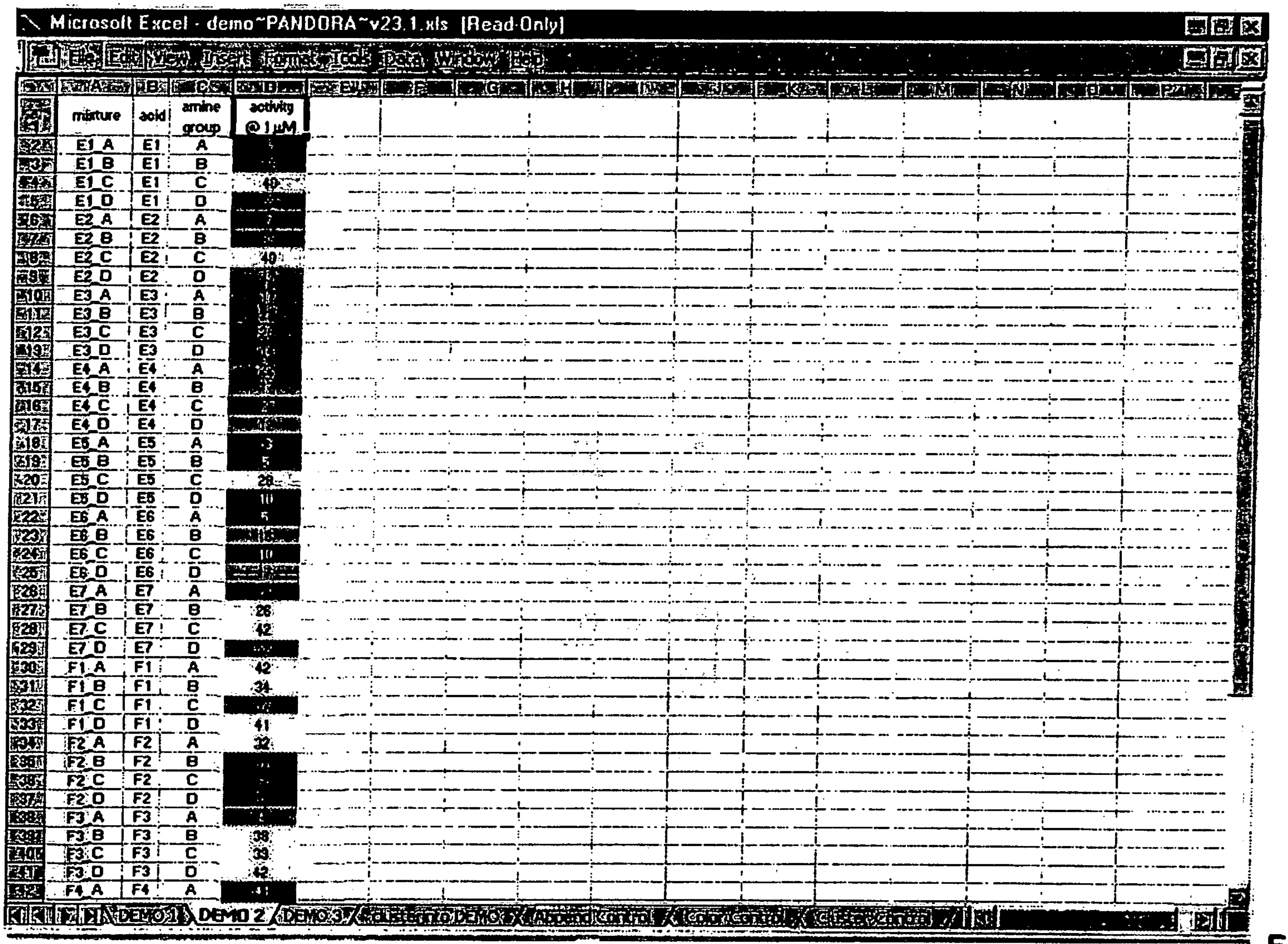
	mixture	acid	amine group	activity @ 1 µM
2	E1_A	E1	A	47
3	E1_B	E1	B	68
4	E1_C	E1	C	40
5	E1_D	E1	D	62
6	E2_A	E2	A	7
7	E2_B	E2	B	69
8	E2_C	E2	C	40
9	E2_D	E2	D	17
10	E3_A	E3	A	17
11	E3_B	E3	B	22
12	E3_C	E3	C	20
13	E3_D	E3	D	14
14	E4_A	E4	A	22
15	E4_B	E4	B	17
16	E4_C	E4	C	-27
17	E4_D	E4	D	12
18	E5_A	E5	A	-3
19	E5_B	E5	B	5
20	E5_C	E5	C	28
21	E5_D	E5	D	10
22	E6_A	E6	A	5
23	E6_B	E6	B	18
24	E6_C	E6	C	10
25	E6_D	E6	D	17
26	E7_A	E7	A	74
27	E7_B	E7	B	26
28	E7_C	E7	C	42
29	E7_D	E7	D	52
30	F1_A	F1	A	42
31	F1_B	F1	B	34
32	F1_C	F1	C	57
33	F1_D	F1	D	41
34	F2_A	F2	A	32
35	F2_B	F2	B	61
36	F2_C	F2	C	72
37	F2_D	F2	D	53
38	F3_A	F3	A	14
39	F3_B	F3	B	38
40	F3_C	F3	C	33
41	F3_D	F3	D	42
42	F4_A	F4	A	-41
43	F4_B	F4	B	9
44	F4_C	F4	C	18

Fig. 9A



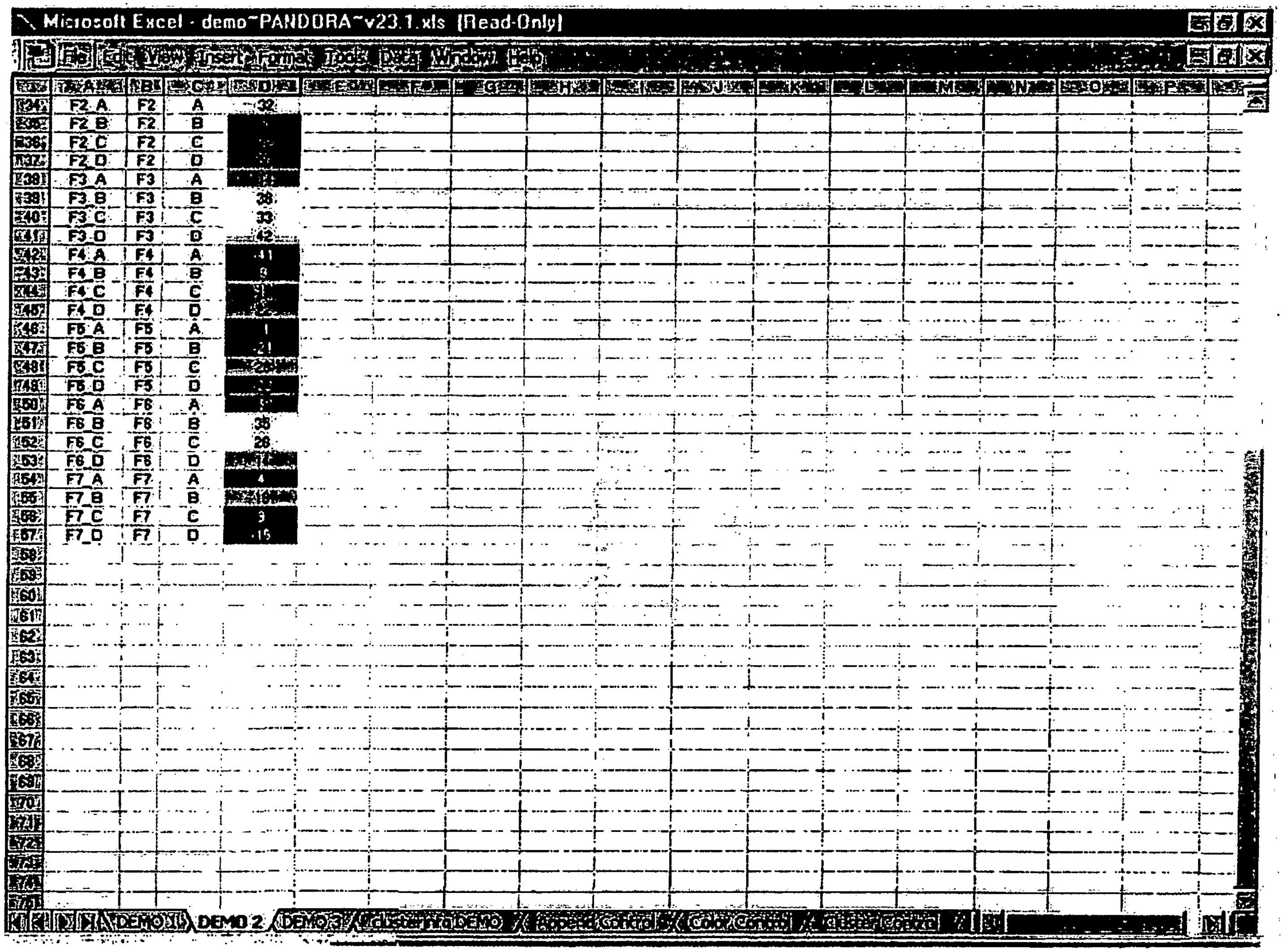
	A	B	C	D
45	F4_D	F4	D	22
46	F5_A	F5	A	-1
47	F5_B	F5	B	-21
48	F5_C	F5	C	23
49	F5_D	F5	D	-22
50	F6_A	F6	A	49
51	F6_B	F6	B	35
52	F6_C	F6	C	26
53	F6_D	F6	D	14
54	F7_A	F7	A	4
55	F7_B	F7	B	19
56	F7_C	F7	C	9
57	F7_D	F7	D	-15

Fig. 9B



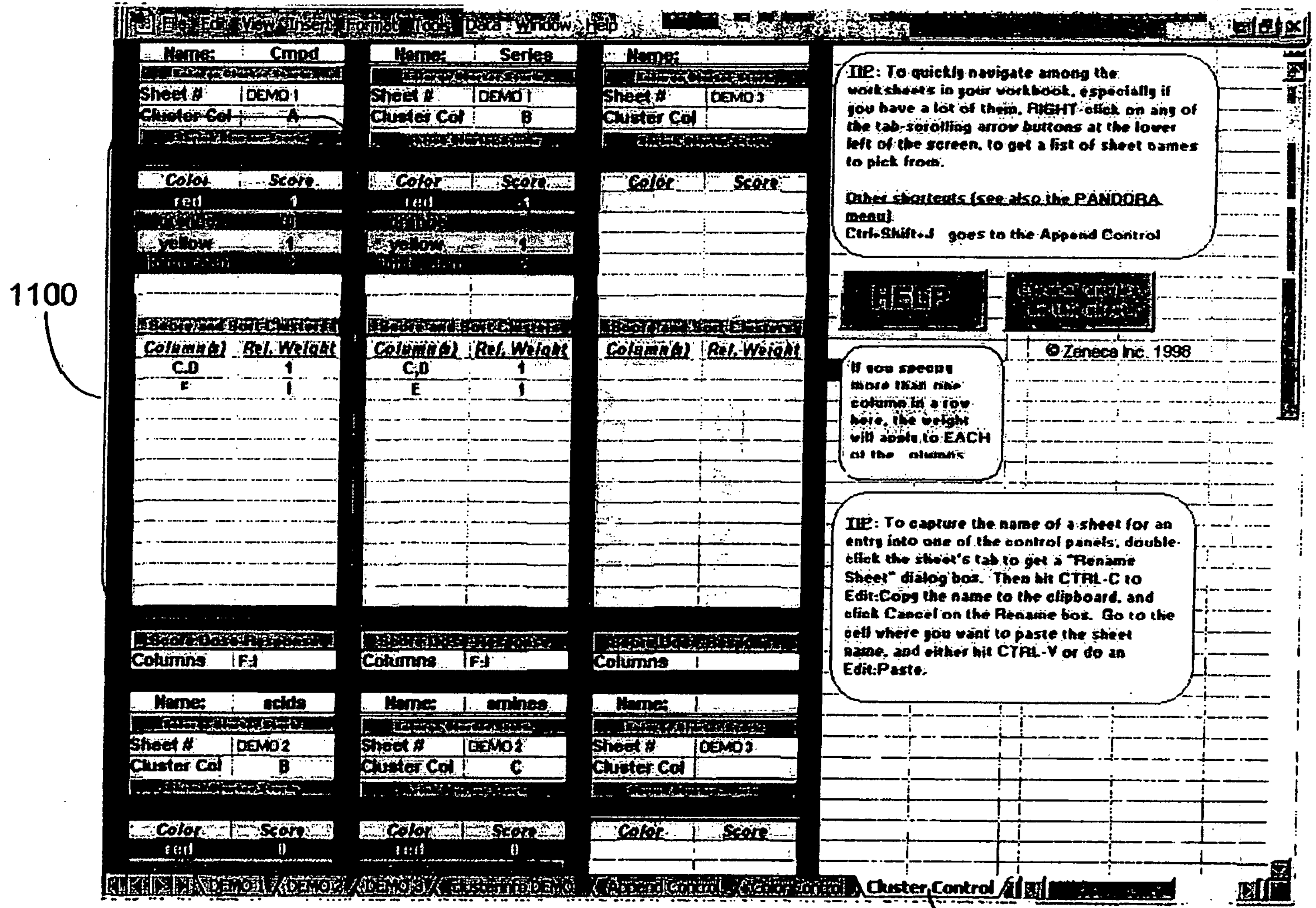
mixture	acid	amine group	activity @ 1 µM
E1_A	E1	A	[illegible]
E1_B	E1	B	[illegible]
E1_C	E1	C	40
E1_D	E1	D	[illegible]
E2_A	E2	A	7
E2_B	E2	B	[illegible]
E2_C	E2	C	40
E2_D	E2	D	[illegible]
E3_A	E3	A	[illegible]
E3_B	E3	B	[illegible]
E3_C	E3	C	[illegible]
E3_D	E3	D	[illegible]
E4_A	E4	A	[illegible]
E4_B	E4	B	[illegible]
E4_C	E4	C	[illegible]
E4_D	E4	D	[illegible]
E5_A	E5	A	3
E5_B	E5	B	5
E5_C	E5	C	28
E5_D	E5	D	10
E6_A	E6	A	5
E6_B	E6	B	16
E6_C	E6	C	10
E6_D	E6	D	[illegible]
E7_A	E7	A	[illegible]
E7_B	E7	B	26
E7_C	E7	C	42
E7_D	E7	D	[illegible]
F1_A	F1	A	42
F1_B	F1	B	34
F1_C	F1	C	[illegible]
F1_D	F1	D	41
F2_A	F2	A	32
F2_B	F2	B	[illegible]
F2_C	F2	C	[illegible]
F2_D	F2	D	[illegible]
F3_A	F3	A	[illegible]
F3_B	F3	B	38
F3_C	F3	C	39
F3_D	F3	D	42
F4_A	F4	A	[illegible]

Fig. 10A



	A	B	C	D
34	F2_A	F2	A	-32
35	F2_B	F2	B	[illegible]
36	F2_C	F2	C	[illegible]
37	F2_D	F2	D	[illegible]
38	F3_A	F3	A	[illegible]
39	F3_B	F3	B	38
40	F3_C	F3	C	33
41	F3_D	F3	D	42
42	F4_A	F4	A	-41
43	F4_B	F4	B	9
44	F4_C	F4	C	[illegible]
45	F4_D	F4	D	[illegible]
46	F5_A	F5	A	1
47	F5_B	F5	B	-21
48	F5_C	F5	C	20
49	F5_D	F5	D	[illegible]
50	F6_A	F6	A	[illegible]
51	F6_B	F6	B	38
52	F6_C	F6	C	28
53	F6_D	F6	D	[illegible]
54	F7_A	F7	A	4
55	F7_B	F7	B	16
56	F7_C	F7	C	9
57	F7_D	F7	D	-15

Fig. 10B



Name:	Cmpd
Sheet #	DEMO 1
Cluster Col	A

Color	Score
red	1
yellow	1

Column(s)	Rel. Weight
C,D	1
F	1

Name:	Series
Sheet #	DEMO 1
Cluster Col	B

Color	Score
red	1
yellow	1

Column(s)	Rel. Weight
C,D	1
E	1

Name:	
Sheet #	DEMO 3
Cluster Col	

Color	Score

Column(s)	Rel. Weight

Columns	F:J
Name:	acids
Sheet #	DEMO 2
Cluster Col	B

Color	Score
red	0

Columns	F:J
Name:	amines
Sheet #	DEMO 2
Cluster Col	C

Color	Score
red	0

Columns	
Name:	
Sheet #	DEMO 3
Cluster Col	

Color	Score

TIP: To quickly navigate among the worksheets in your workbook, especially if you have a lot of them, RIGHT-click on any of the tab-scrolling arrow buttons at the lower left of the screen, to get a list of sheet names to pick from.

Other shortcuts (see also the PANDORA menu)
Ctrl+Shift+J goes to the Append Control

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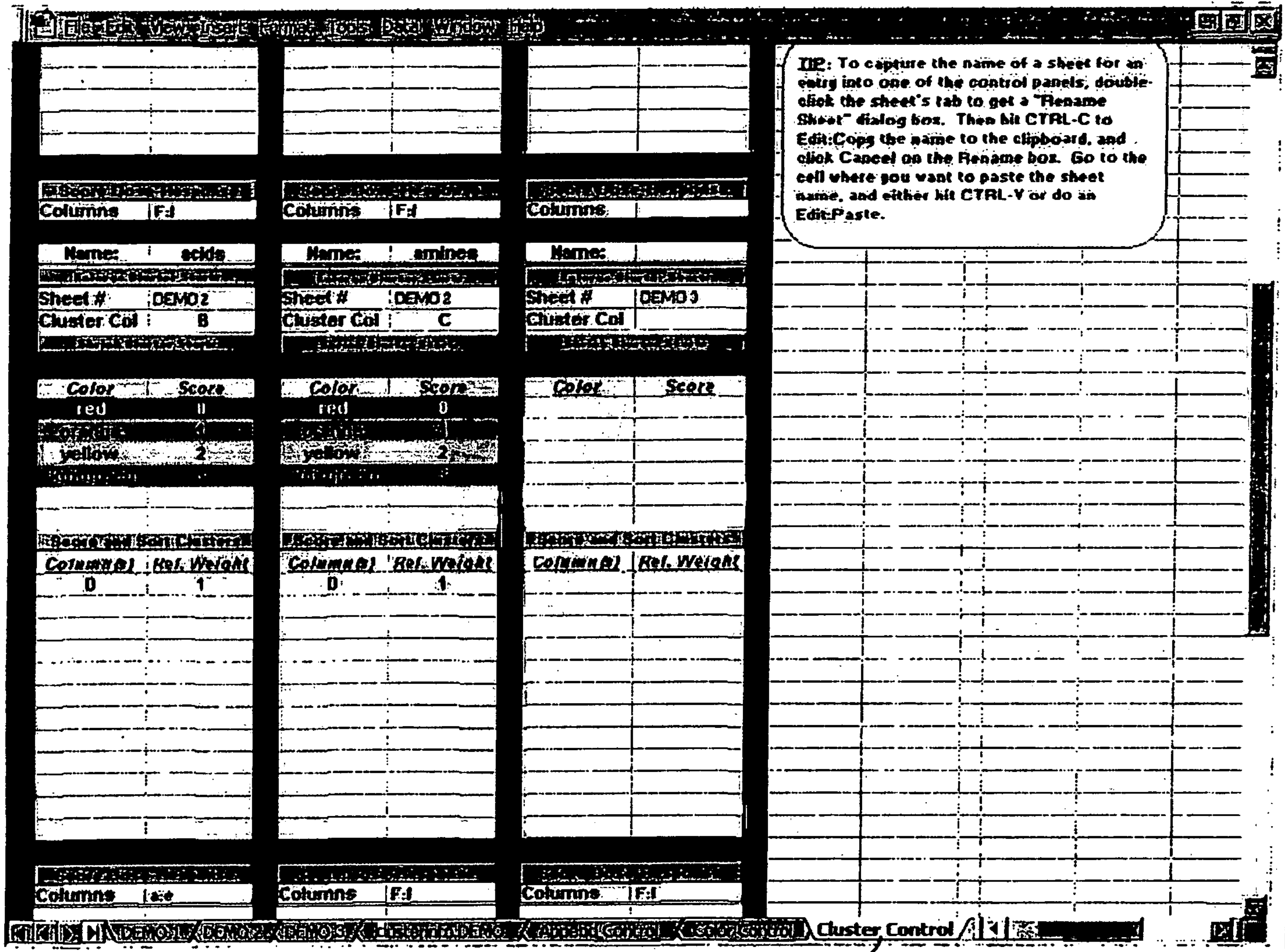
If you specify more than one column in a row here, the weight will apply to EACH of the columns

TIP: To capture the name of a sheet for an entry into one of the control panels, double-click the sheet's tab to get a "Rename Sheet" dialog box. Then hit CTRL-C to Edit:Copy the name to the clipboard, and click Cancel on the Rename box. Go to the cell where you want to paste the sheet name, and either hit CTRL-V or do an Edit:Paste.

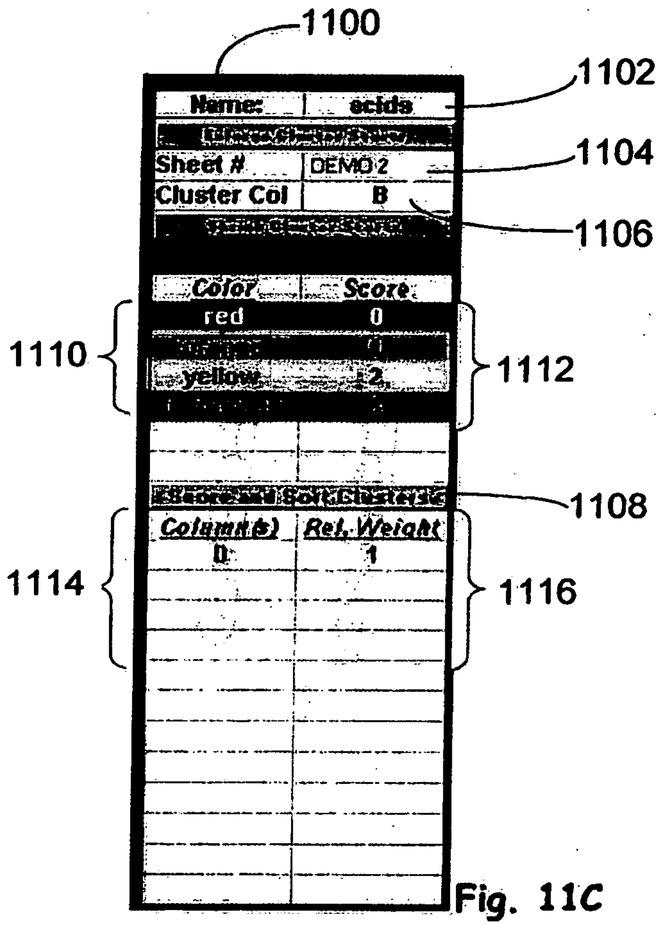
Fig. 11A



Columns	F:I	Columns	F:I	Columns	
Name:	acids	Name:	amines	Name:	
Sheet #	DEMO 2	Sheet #	DEMO 2	Sheet #	DEMO 3
Cluster Col	B	Cluster Col	C	Cluster Col	
Color	*Score*	*Color*	*Score*	*Color*	*Score*
red	0	red	0		
yellow	2	yellow	2		
Column(s)	*Rel. Weight*	*Column(s)*	*Rel. Weight*	*Column(s)*	*Rel. Weight*
D	1	D	1		
Columns	a:e	Columns	F:I	Columns	F:I

TIP: To capture the name of a sheet for an entry into one of the control panels, double-click the sheet's tab to get a "Rename Sheet" dialog box. Then hit CTRL-C to Edit:Copy the name to the clipboard, and click Cancel on the Rename box. Go to the cell where you want to paste the sheet name, and either hit CTRL-V or do an Edit:Paste.

Fig. 11B

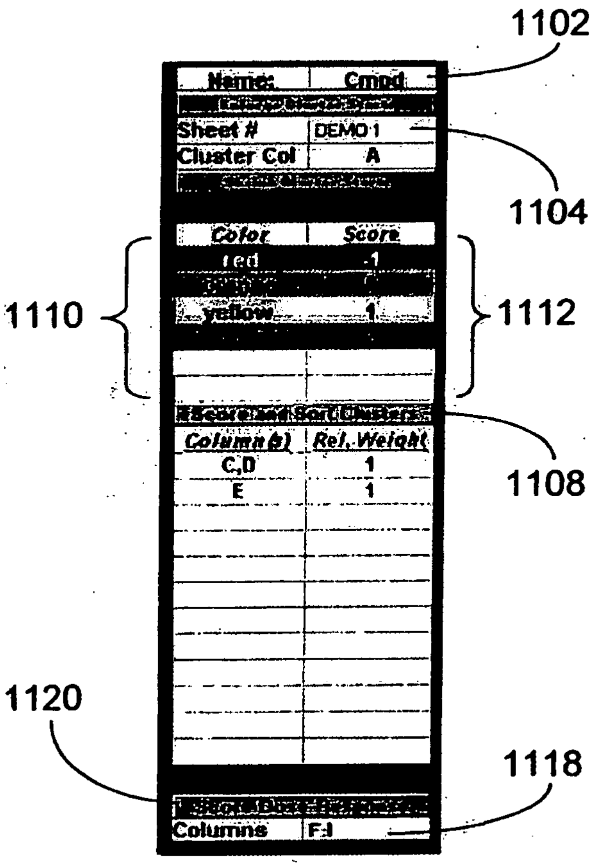


Name:	acids
Sheet #	DEMO 2
Cluster Col	B

Color	Score
red	0
[illegible]	1
yellow	2
[illegible]	[illegible]

Column(s)	Rel. Weight
D	1

Fig. 11C



Name:	Cmpd
[illegible]	
Sheet #	DEMO1
Cluster Col	A
[illegible]	

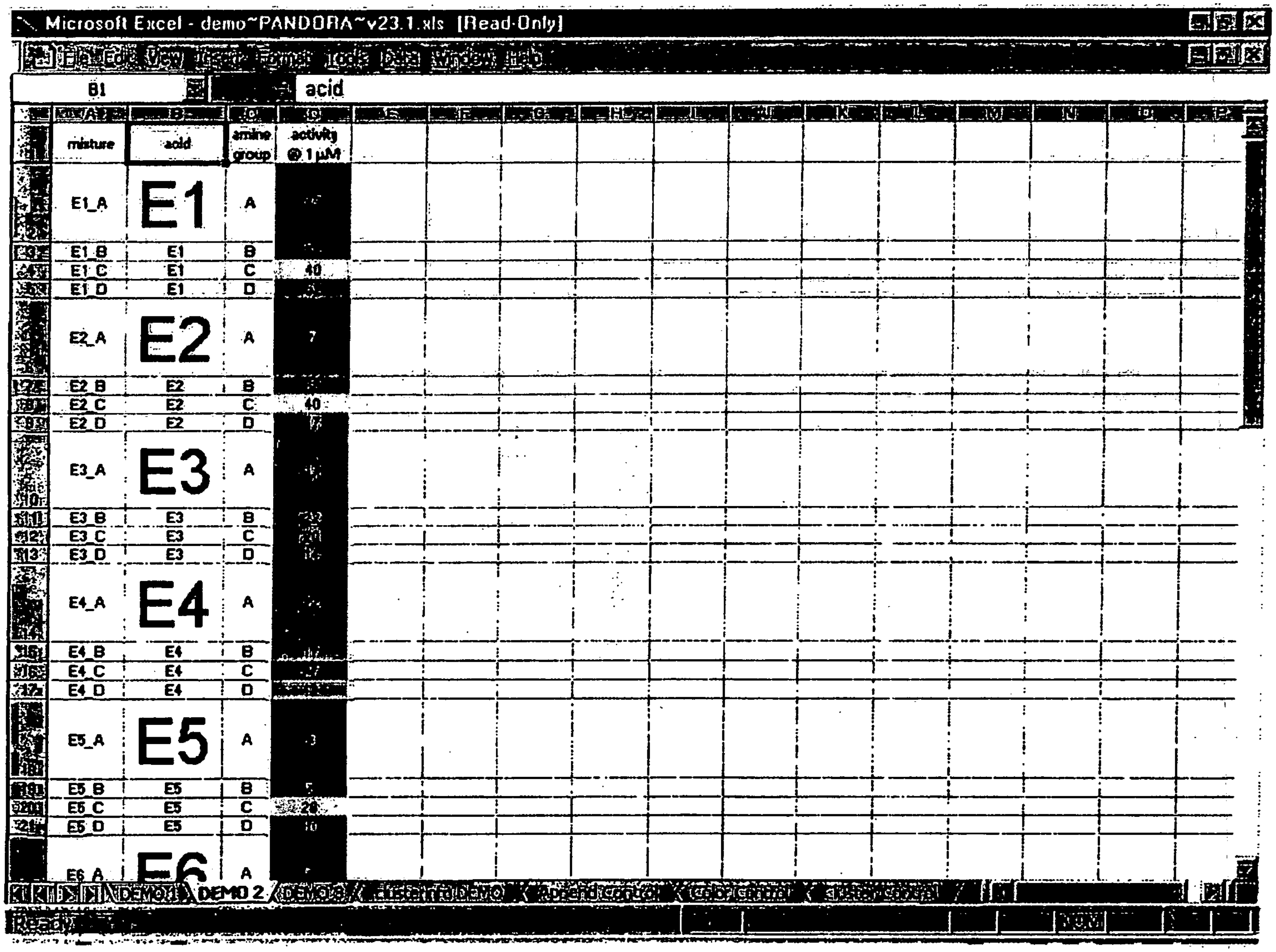
Color	Score
red	-1
[illegible]	[illegible]
yellow	1

Score and Sort Clusters

Column(s)	Rel. Weight
C,D	1
E	1

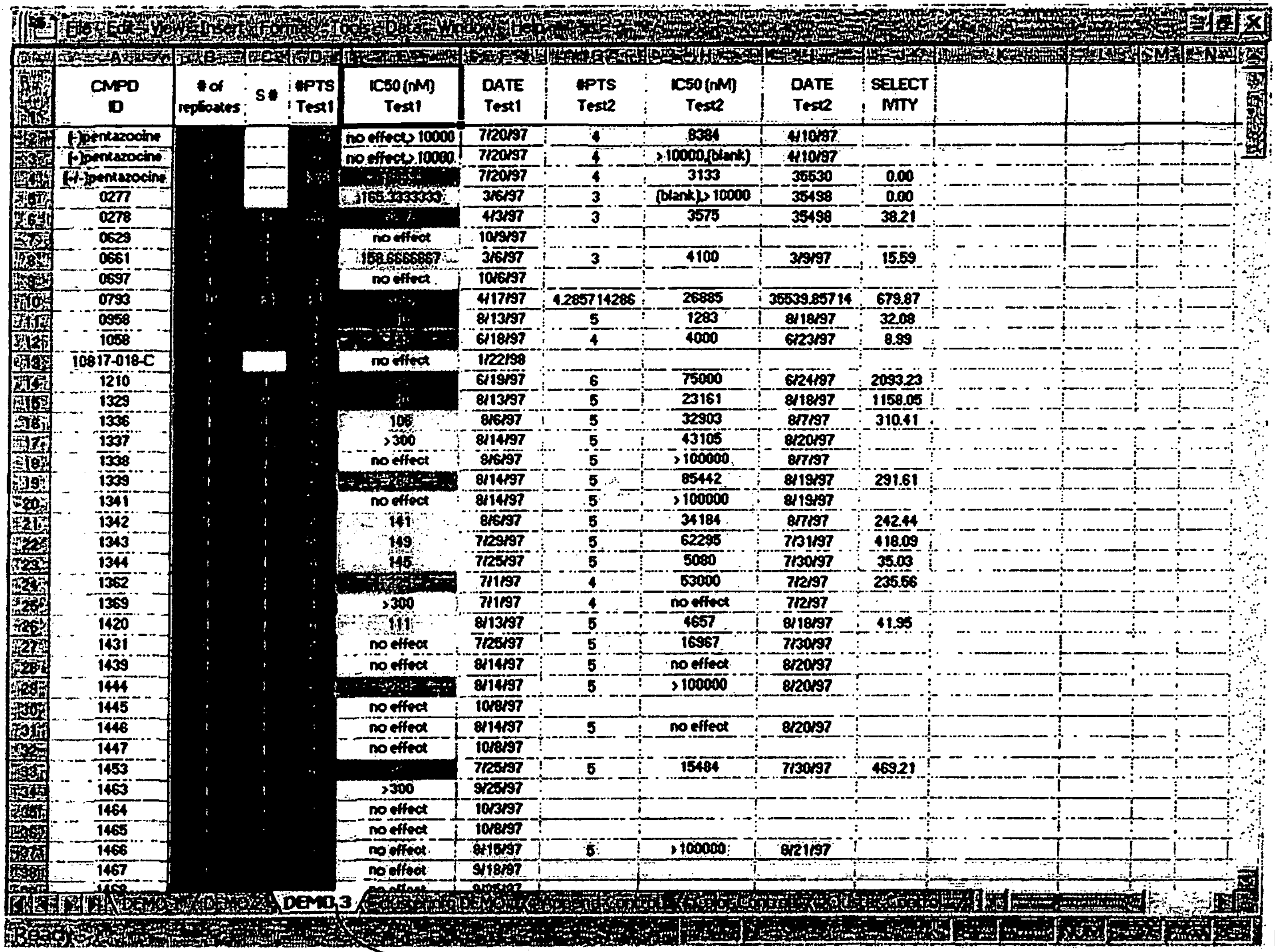
[illegible]	
Columns	F:I

Fig. 11D



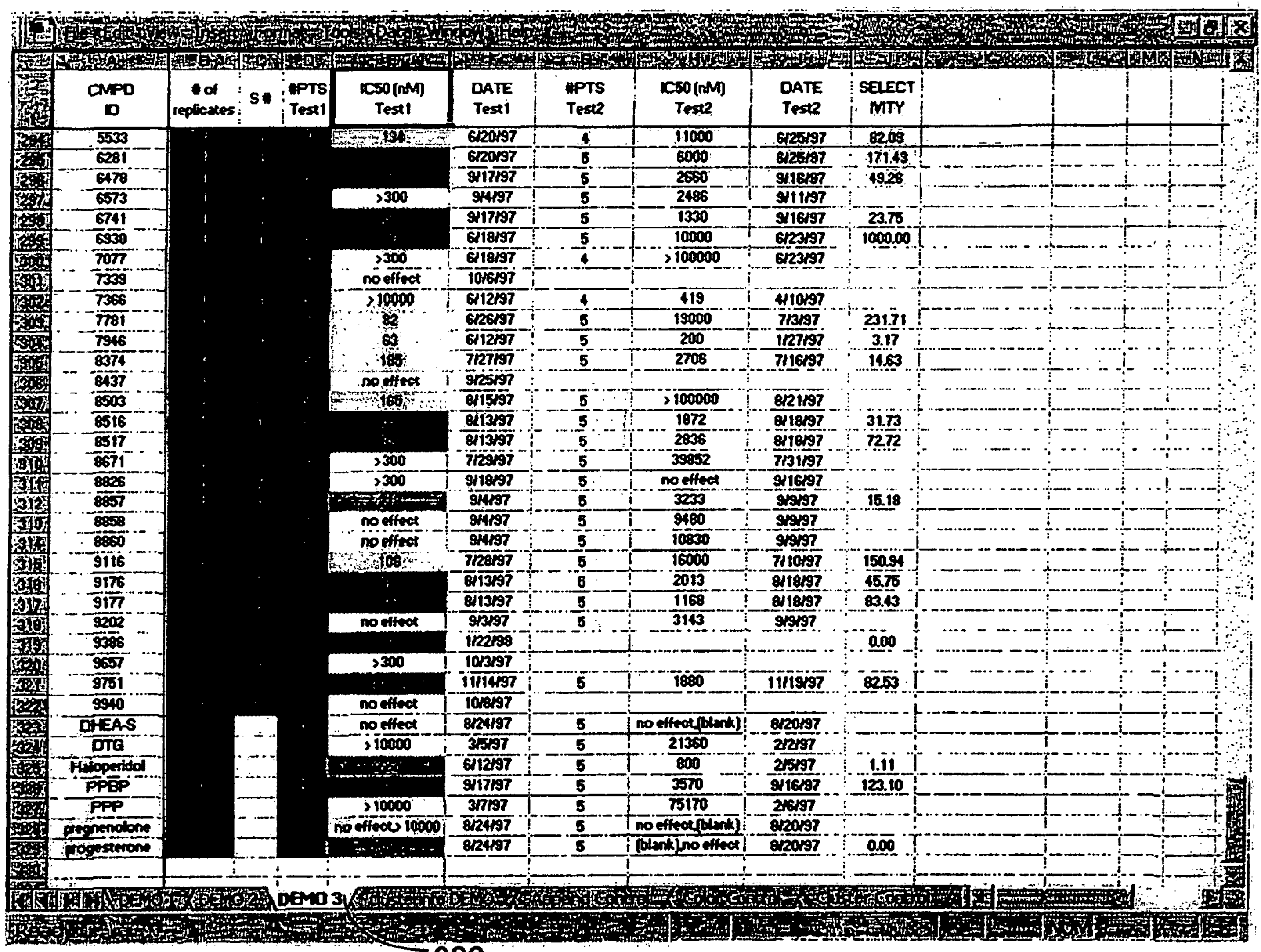
mixture	acid	amine group	activity @ 1 µM
E1_A	E1	A	[illegible]
E1_B	E1	B	[illegible]
E1_C	E1	C	40
E1_D	E1	D	[illegible]
E2_A	E2	A	7
E2_B	E2	B	[illegible]
E2_C	E2	C	40
E2_D	E2	D	[illegible]
E3_A	E3	A	[illegible]
E3_B	E3	B	[illegible]
E3_C	E3	C	[illegible]
E3_D	E3	D	[illegible]
E4_A	E4	A	[illegible]
E4_B	E4	B	[illegible]
E4_C	E4	C	[illegible]
E4_D	E4	D	[illegible]
E5_A	E5	A	3
E5_B	E5	B	5
E5_C	E5	C	20
E5_D	E5	D	10
E6_A	E6	A	[illegible]

Fig. 12



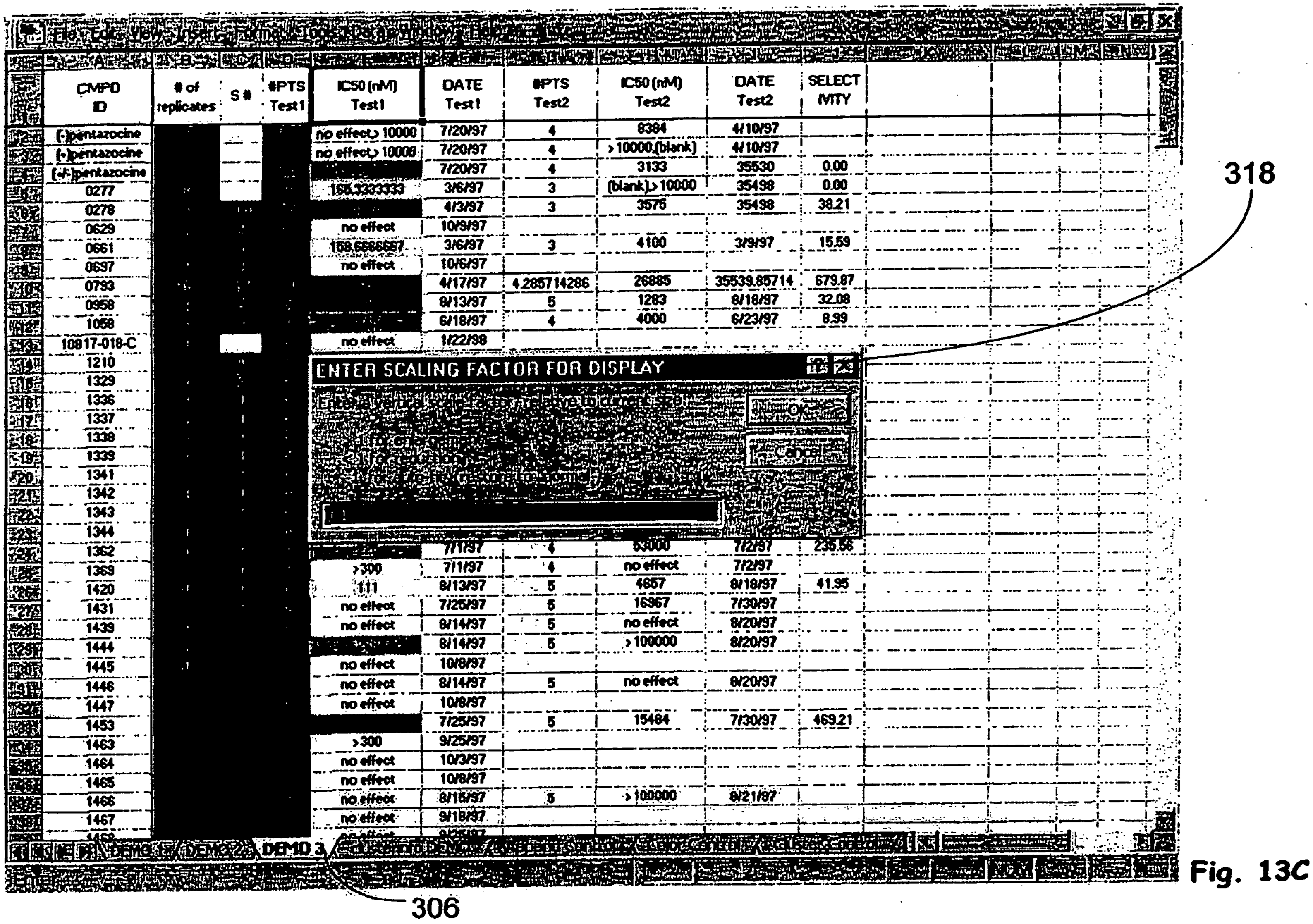
CMPD ID	# of replicates	S #	#PTS Test1	IC50 (nM) Test1	DATE Test1	#PTS Test2	IC50 (nM) Test2	DATE Test2	SELECTIVITY
(-)pentazocine	[redacted]		[redacted]	no effect,> 10000	7/20/97	4	8384	4/10/97	
(+)pentazocine	[redacted]		[redacted]	no effect,> 10000	7/20/97	4	>10000,(blank)	4/10/97	
(+/-)pentazocine	[redacted]		[redacted]	[redacted]	7/20/97	4	3133	35530	0.00
0277	[redacted]		[redacted]	165.3333333	3/6/97	3	(blank),> 10000	35498	0.00
0278	[redacted]	[redacted]	[redacted]	[redacted]	4/3/97	3	3575	35498	38.21
0629	[redacted]	[redacted]	[redacted]	no effect	10/9/97				
0661	[redacted]	[redacted]	[redacted]	158.6666667	3/6/97	3	4100	3/9/97	15.59
0697	[redacted]	[redacted]	[redacted]	no effect	10/6/97				
0793	[redacted]	[redacted]	[redacted]	[redacted]	4/17/97	4.285714286	26885	35539.85714	679.87
0958	[redacted]	[redacted]	[redacted]	[redacted]	8/13/97	5	1283	8/18/97	32.08
1058	[redacted]	[redacted]	[redacted]	[redacted]	6/18/97	4	4000	6/23/97	8.99
10817-018-C	[redacted]		[redacted]	no effect	1/22/98				
1210	[redacted]	[redacted]	[redacted]	[redacted]	6/19/97	6	75000	6/24/97	2093.23
1329	[redacted]	[redacted]	[redacted]	[redacted]	8/13/97	5	23161	8/18/97	1158.05
1336	[redacted]	[redacted]	[redacted]	106	8/6/97	5	32903	8/7/97	310.41
1337	[redacted]	[redacted]	[redacted]	>300	8/14/97	5	43105	8/20/97	
1338	[redacted]	[redacted]	[redacted]	no effect	8/6/97	5	>100000	8/7/97	
1339	[redacted]	[redacted]	[redacted]	[redacted]	8/14/97	5	85442	8/19/97	291.61
1341	[redacted]	[redacted]	[redacted]	no effect	8/14/97	5	>100000	8/19/97	
1342	[redacted]	[redacted]	[redacted]	141	8/6/97	5	34184	8/7/97	242.44
1343	[redacted]	[redacted]	[redacted]	149	7/29/97	5	62295	7/31/97	418.09
1344	[redacted]	[redacted]	[redacted]	145	7/25/97	5	5080	7/30/97	35.03
1362	[redacted]	[redacted]	[redacted]	[redacted]	7/1/97	4	53000	7/2/97	235.56
1369	[redacted]	[redacted]	[redacted]	>300	7/1/97	4	no effect	7/2/97	
1420	[redacted]	[redacted]	[redacted]	111	8/13/97	5	4657	8/18/97	41.95
1431	[redacted]	[redacted]	[redacted]	no effect	7/25/97	5	16967	7/30/97	
1439	[redacted]	[redacted]	[redacted]	no effect	8/14/97	5	no effect	8/20/97	
1444	[redacted]	[redacted]	[redacted]	[redacted]	8/14/97	5	>100000	8/20/97	
1445	[redacted]	[redacted]	[redacted]	no effect	10/8/97				
1446	[redacted]	[redacted]	[redacted]	no effect	8/14/97	5	no effect	8/20/97	
1447	[redacted]	[redacted]	[redacted]	no effect	10/8/97				
1453	[redacted]	[redacted]	[redacted]	[redacted]	7/25/97	5	15484	7/30/97	469.21
1463	[redacted]	[redacted]	[redacted]	>300	9/25/97				
1464	[redacted]	[redacted]	[redacted]	no effect	10/3/97				
1465	[redacted]	[redacted]	[redacted]	no effect	10/8/97				
1466	[redacted]	[redacted]	[redacted]	no effect	8/15/97	5	>100000	8/21/97	
1467	[redacted]	[redacted]	[redacted]	no effect	9/18/97				

Fig. 13A



CMPD ID	# of replicates	S #	#PTS Test1	IC50 (nM) Test1	DATE Test1	#PTS Test2	IC50 (nM) Test2	DATE Test2	SELECT IVITY
5533				134	6/20/97	4	11000	6/25/97	82.09
6281					6/20/97	5	6000	6/25/97	171.43
6478					9/17/97	5	2660	9/16/97	49.26
6573				>300	9/4/97	5	2486	9/11/97	
6741					9/17/97	5	1330	9/16/97	23.75
6930					6/18/97	5	10000	6/23/97	1000.00
7077				>300	6/18/97	4	>100000	6/23/97	
7339				no effect	10/6/97				
7366				>10000	6/12/97	4	419	4/10/97	
7781				82	6/26/97	5	19000	7/3/97	231.71
7946				63	6/12/97	5	200	1/27/97	3.17
8374				185	7/27/97	5	2706	7/16/97	14.63
8437				no effect	9/25/97				
8503				166	8/15/97	5	>100000	8/21/97	
8516					8/13/97	5	1872	8/18/97	31.73
8517					8/13/97	5	2836	8/18/97	72.72
8671				>300	7/29/97	5	39852	7/31/97	
8826				>300	9/18/97	5	no effect	9/16/97	
8857					9/4/97	5	3233	9/9/97	15.18
8858				no effect	9/4/97	5	9480	9/9/97	
8860				no effect	9/4/97	5	10830	9/9/97	
9116				108	7/28/97	5	16000	7/10/97	150.94
9176					8/13/97	5	2013	8/18/97	45.75
9177					8/13/97	5	1168	8/18/97	83.43
9202				no effect	9/3/97	5	3143	9/9/97	
9386					1/22/98				0.00
9657				>300	10/3/97				
9751					11/14/97	5	1880	11/19/97	82.53
9940				no effect	10/8/97				
DHEA-S				no effect	8/24/97	5	no effect,(blank)	8/20/97	
DTG				>10000	3/5/97	5	21360	2/2/97	
Haloperidol					6/12/97	5	800	2/5/97	1.11
PPBP					9/17/97	5	3570	9/16/97	123.10
PPP				>10000	3/7/97	5	75170	2/6/97	
pregnenolone				no effect,>10000	8/24/97	5	no effect,(blank)	8/20/97	
progesterone					8/24/97	5	(blank),no effect	8/20/97	0.00

Fig. 13B



CMPD ID	# of replicates	S #	#PTS Test1	IC50 (nM) Test1	DATE Test1	#PTS Test2	IC50 (nM) Test2	DATE Test2	SELECTIVITY
(-)pentazocine				no effect,> 10000	7/20/97	4	8384	4/10/97	
(-)pentazocine				no effect,> 10000	7/20/97	4	> 10000,(blank)	4/10/97	
(+/-)pentazocine					7/20/97	4	3133	35530	0.00
0277				166.3333333	3/6/97	3	(blank),> 10000	35498	0.00
0278					4/3/97	3	3576	35498	38.21
0629				no effect	10/9/97				
0661				158.6666667	3/6/97	3	4100	3/9/97	15.59
0697				no effect	10/6/97				
0793					4/17/97	4.285714286	26885	35539.85714	679.87
0958					8/13/97	5	1283	8/18/97	32.08
1058					6/18/97	4	4000	6/23/97	8.99
10817-018-C				no effect	1/22/98				
1210									
1329									
1336									
1337									
1338									
1339									
1341									
1342									
1343									
1344									
1362					7/1/97	4	53000	7/2/97	235.56
1369				>300	7/1/97	4	no effect	7/2/97	
1420				111	8/13/97	5	4657	8/18/97	41.95
1431				no effect	7/25/97	5	16967	7/30/97	
1439				no effect	8/14/97	5	no effect	8/20/97	
1444					8/14/97	5	>100000	8/20/97	
1445				no effect	10/8/97				
1446				no effect	8/14/97	5	no effect	8/20/97	
1447				no effect	10/8/97				
1453					7/25/97	5	15484	7/30/97	469.21
1463				>300	9/25/97				
1464				no effect	10/3/97				
1465				no effect	10/8/97				
1466				no effect	8/15/97	5	>100000	8/21/97	
1467				no effect	9/18/97				

Fig. 13C

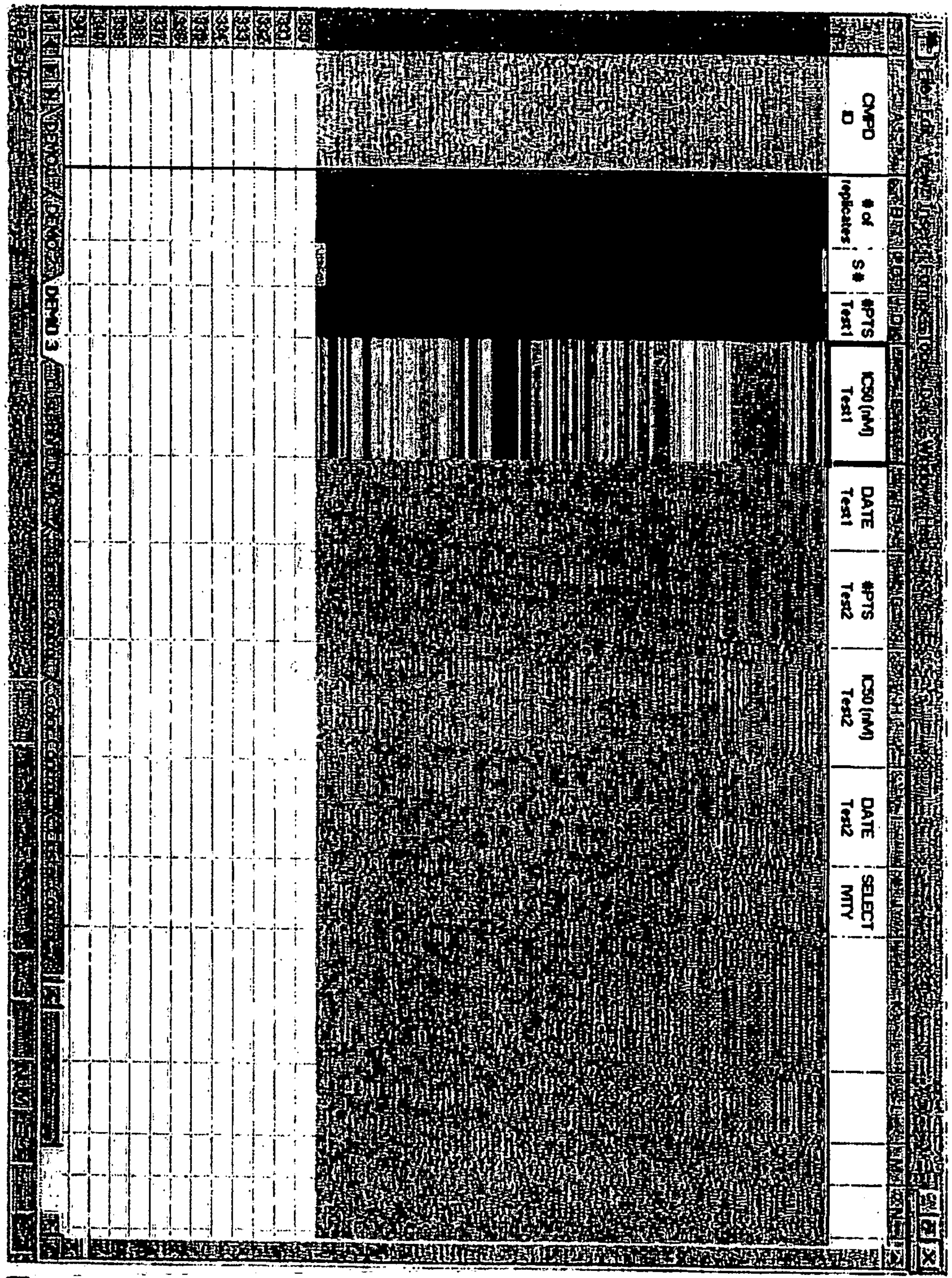
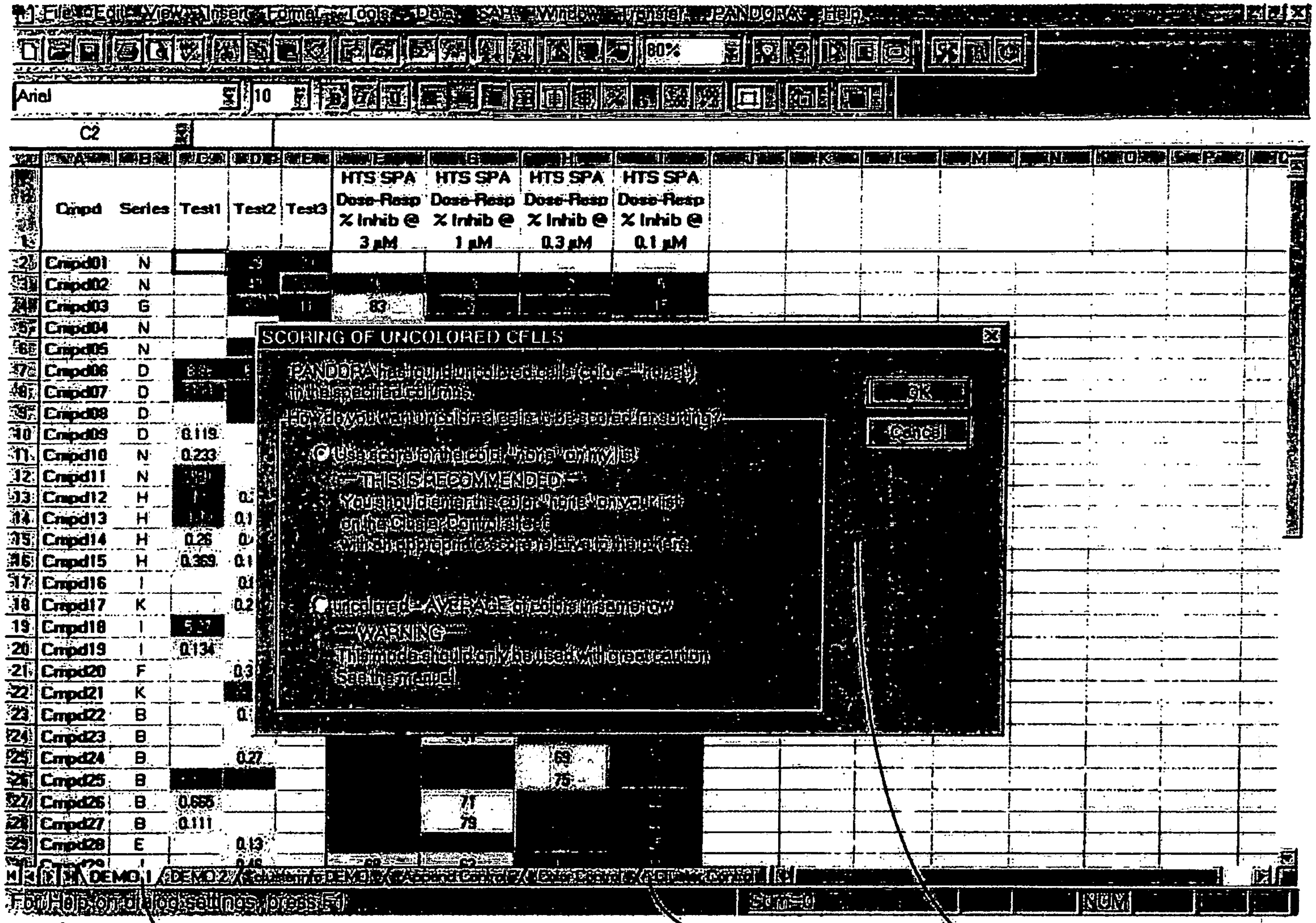

CMPD ID
# of replicates
S#
#PTS Test1
IC50 (nM) Test1
DATE Test1
#PTS Test2
IC50 (nM) Test2
DATE Test2
SELECT MTY
DEMO 3

Fig. 13D



Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3 µM	HTS SPA Dose-Resp % Inhib @ 1 µM	HTS SPA Dose-Resp % Inhib @ 0.3 µM	HTS SPA Dose-Resp % Inhib @ 0.1 µM
Cmpd01	N							
Cmpd02	N							
Cmpd03	G				83			
Cmpd04	N							
Cmpd05	N							
Cmpd06	D							
Cmpd07	D							
Cmpd08	D							
Cmpd09	D	0.119						
Cmpd10	N	0.233						
Cmpd11	N							
Cmpd12	H		0.					
Cmpd13	H		0.1					
Cmpd14	H	0.26	0.					
Cmpd15	H	0.369	0.1					
Cmpd16	I		0.1					
Cmpd17	K		0.2					
Cmpd18	I							
Cmpd19	I	0.134						
Cmpd20	F		0.3					
Cmpd21	K							
Cmpd22	B		0.					
Cmpd23	B							
Cmpd24	B		0.27				69	
Cmpd25	B						75	
Cmpd26	B	0.665				71		
Cmpd27	B	0.111				79		
Cmpd28	E		0.13					

SCORING OF UNCOLORED CELLS

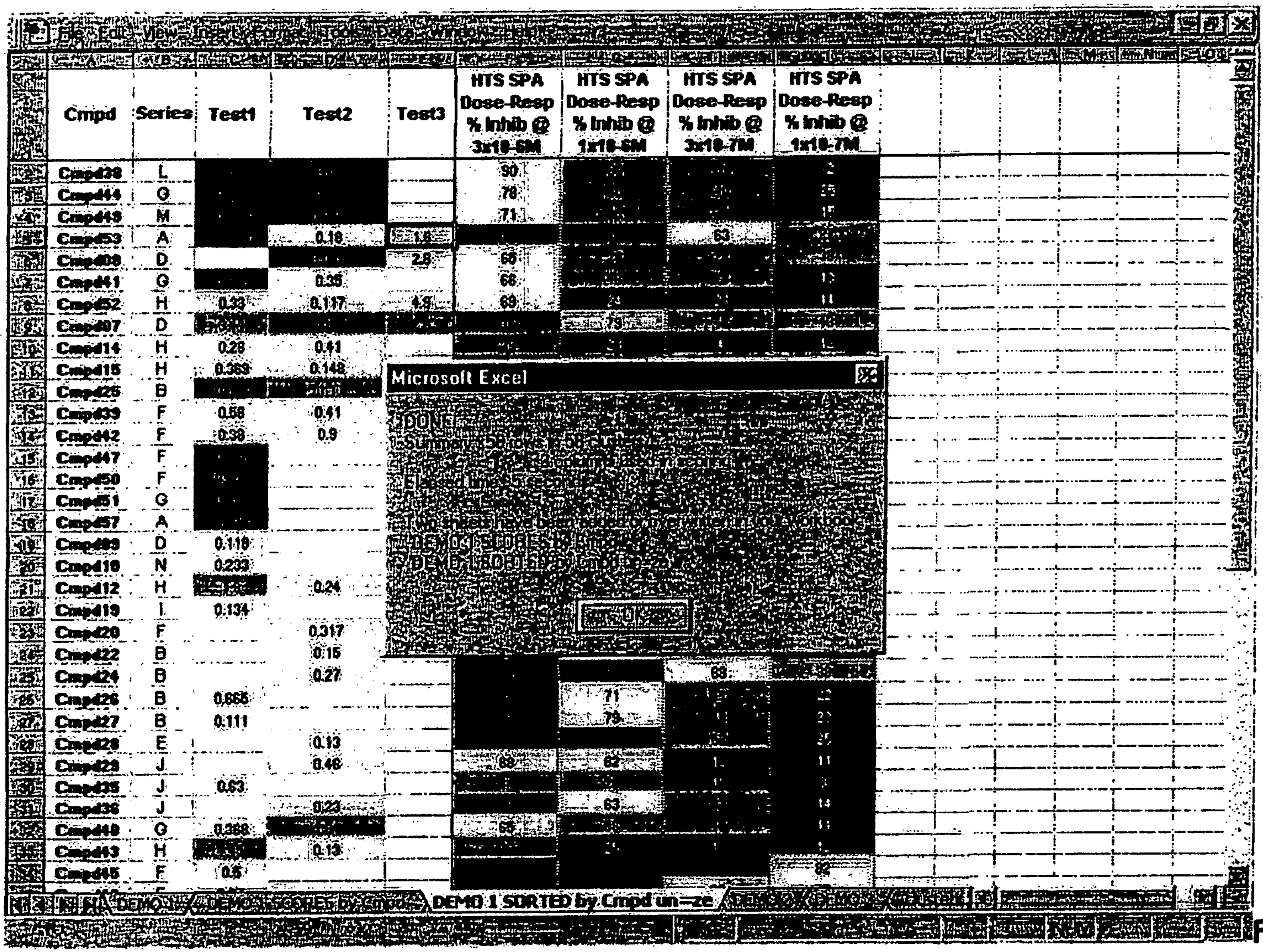
PANDORA has found uncolored cells (color = "none") in the specified columns.

How do you want uncolored cells to be scored for sorting?

○ Use score for the color "none" on my list
<-- THIS IS RECOMMENDED -->
You should enter the color "none" on your list
on the Color Control sheet
with an appropriate score relative to the others.

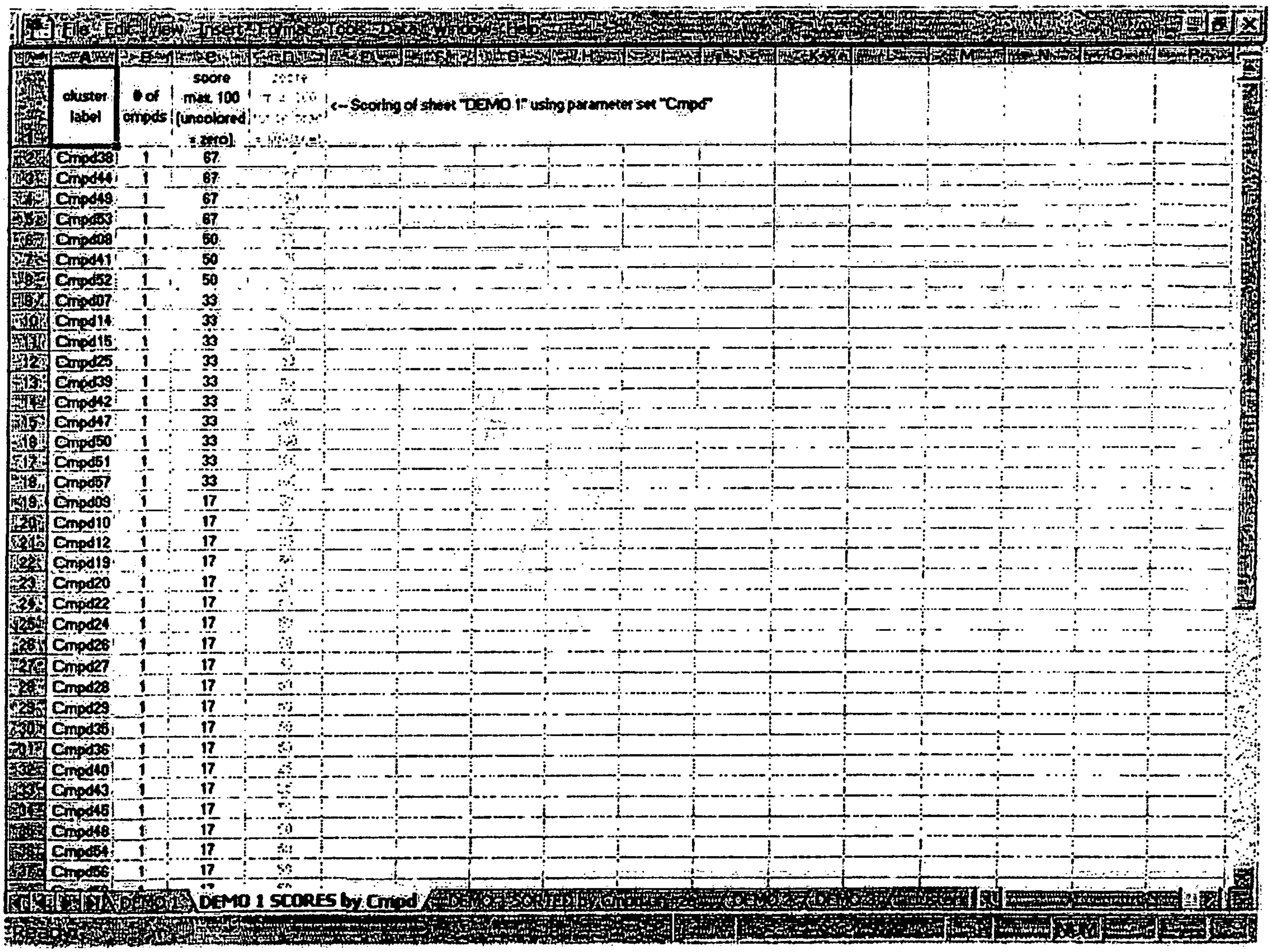
○ uncolored = AVERAGE of colors in same row
--- WARNING ---
This mode should only be used with great caution
See the manual.

Fig. 14A



	Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
2	Cmpd38	L	[illegible]	[illegible]		90	[illegible]	[illegible]	[illegible]
3	Cmpd44	G	[illegible]	[illegible]		78	[illegible]	[illegible]	[illegible]
4	Cmpd49	M	[illegible]	[illegible]		71	[illegible]	[illegible]	[illegible]
5	Cmpd53	A	[illegible]	0.18	1.6	[illegible]	[illegible]	63	[illegible]
6	Cmpd08	D		[illegible]	2.8	60	[illegible]	[illegible]	[illegible]
7	Cmpd41	G	[illegible]	0.35		66	[illegible]	[illegible]	[illegible]
8	Cmpd52	H	0.33	0.117	4.9	69	24	21	11
9	Cmpd07	D	[illegible]	[illegible]	[illegible]	[illegible]	79	[illegible]	[illegible]
10	Cmpd14	H	0.28	0.41		[illegible]	[illegible]	[illegible]	[illegible]
11	Cmpd15	H	0.363	0.148					
12	Cmpd25	B	[illegible]	[illegible]					
13	Cmpd39	F	0.58	0.41					
14	Cmpd42	F	0.38	0.9					
15	Cmpd47	F	[illegible]						
16	Cmpd50	F	[illegible]						
17	Cmpd51	G	[illegible]						
18	Cmpd57	A	[illegible]						
19	Cmpd09	D	0.118						
20	Cmpd10	N	0.233						
21	Cmpd12	H	[illegible]	0.24					
22	Cmpd19	I	0.134						
23	Cmpd20	F		0.317					
24	Cmpd22	B		0.15					
25	Cmpd24	B		0.27		[illegible]	[illegible]	69	[illegible]
26	Cmpd26	B	0.665			[illegible]	71	[illegible]	[illegible]
27	Cmpd27	B	0.111			[illegible]	79	[illegible]	[illegible]
28	Cmpd28	E		0.13		[illegible]	[illegible]	[illegible]	[illegible]
29	Cmpd29	J		0.46		68	62	[illegible]	11
30	Cmpd35	J	0.63			[illegible]	[illegible]	[illegible]	[illegible]
31	Cmpd36	J		0.23		[illegible]	63	[illegible]	14
32	Cmpd40	G	0.388	[illegible]		65	[illegible]	[illegible]	11
33	Cmpd43	H	[illegible]	0.13		[illegible]	[illegible]	1	[illegible]
34	Cmpd45	F	0.5			[illegible]	[illegible]	[illegible]	82

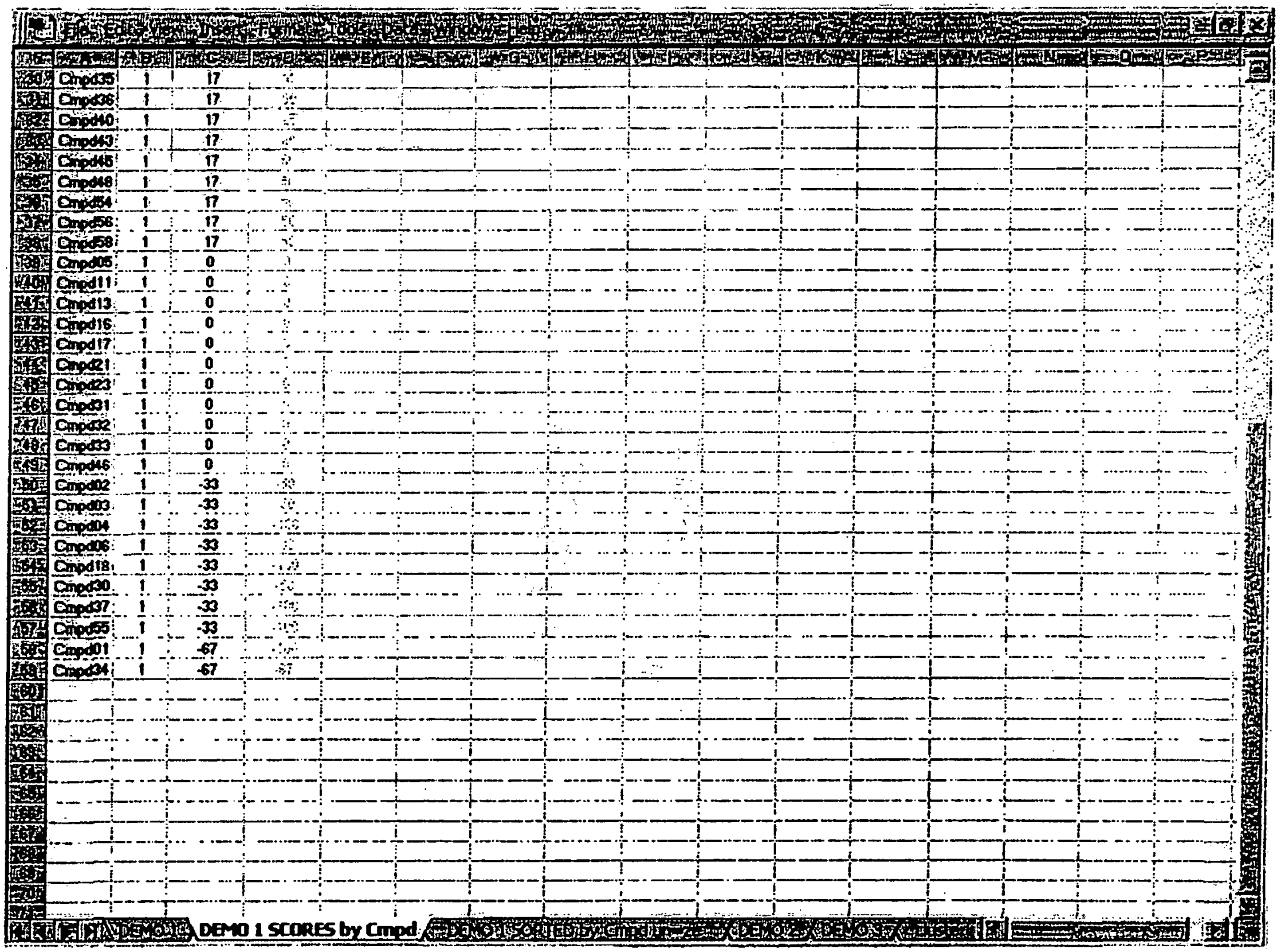
Fig. 14B



<-- Scoring of sheet "DEMO 1" using parameter set "Cmpd"

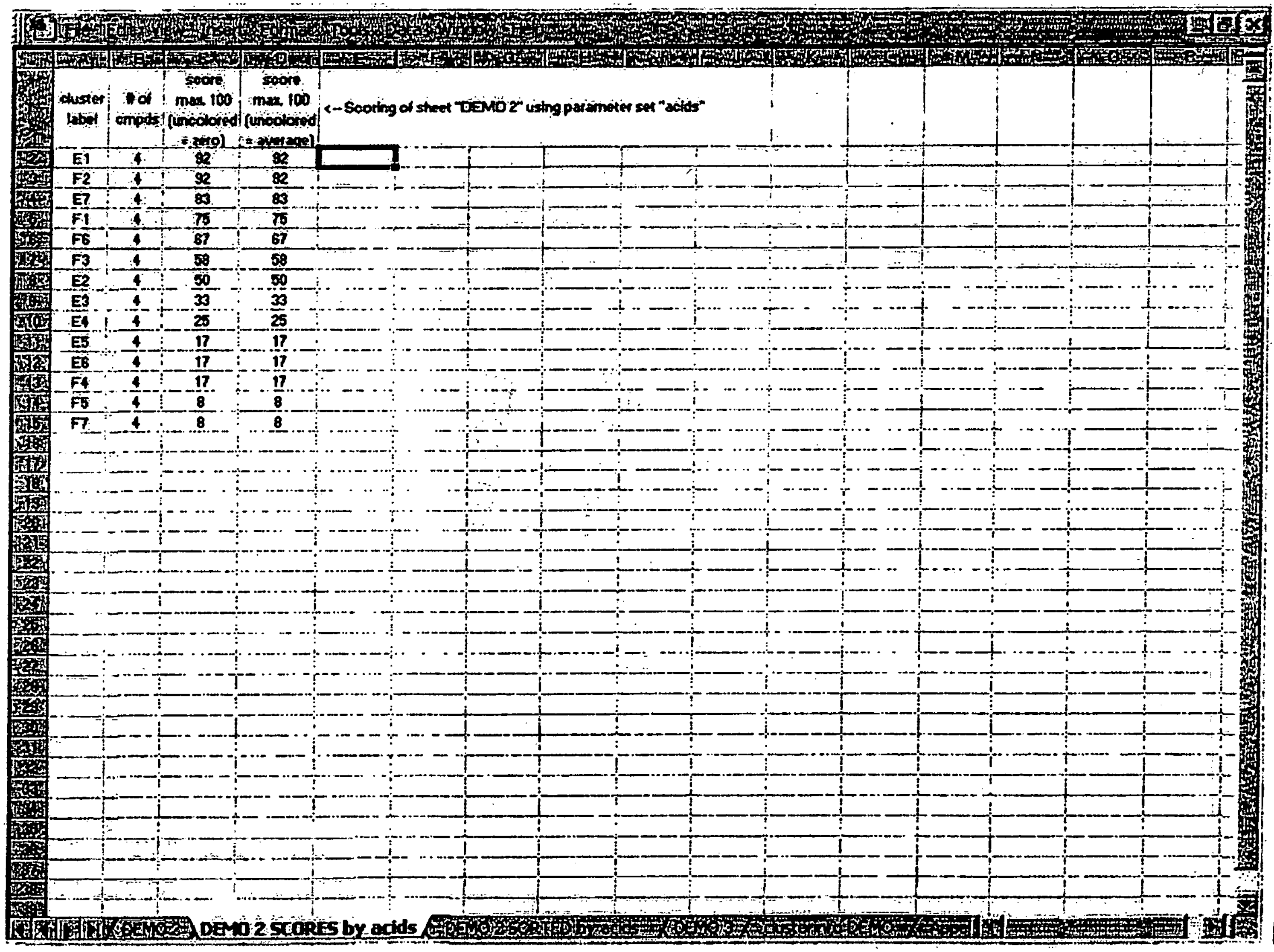
cluster label	# of cmpds	score max. 100 [uncolored = zero]
Cmpd38	1	67
Cmpd44	1	67
Cmpd49	1	67
Cmpd53	1	67
Cmpd08	1	50
Cmpd41	1	50
Cmpd52	1	50
Cmpd07	1	33
Cmpd14	1	33
Cmpd15	1	33
Cmpd25	1	33
Cmpd39	1	33
Cmpd42	1	33
Cmpd47	1	33
Cmpd50	1	33
Cmpd51	1	33
Cmpd57	1	33
Cmpd09	1	17
Cmpd10	1	17
Cmpd12	1	17
Cmpd19	1	17
Cmpd20	1	17
Cmpd22	1	17
Cmpd24	1	17
Cmpd26	1	17
Cmpd27	1	17
Cmpd28	1	17
Cmpd29	1	17
Cmpd35	1	17
Cmpd36	1	17
Cmpd40	1	17
Cmpd43	1	17
Cmpd45	1	17
Cmpd48	1	17
Cmpd54	1	17
Cmpd56	1	17

Fig. 14C



Cmpd35	1	17
Cmpd36	1	17
Cmpd40	1	17
Cmpd43	1	17
Cmpd45	1	17
Cmpd48	1	17
Cmpd54	1	17
Cmpd56	1	17
Cmpd58	1	17
Cmpd05	1	0
Cmpd11	1	0
Cmpd13	1	0
Cmpd16	1	0
Cmpd17	1	0
Cmpd21	1	0
Cmpd23	1	0
Cmpd31	1	0
Cmpd32	1	0
Cmpd33	1	0
Cmpd46	1	0
Cmpd02	1	-33
Cmpd03	1	-33
Cmpd04	1	-33
Cmpd06	1	-33
Cmpd18	1	-33
Cmpd30	1	-33
Cmpd37	1	-33
Cmpd55	1	-33
Cmpd01	1	-67
Cmpd34	1	-67

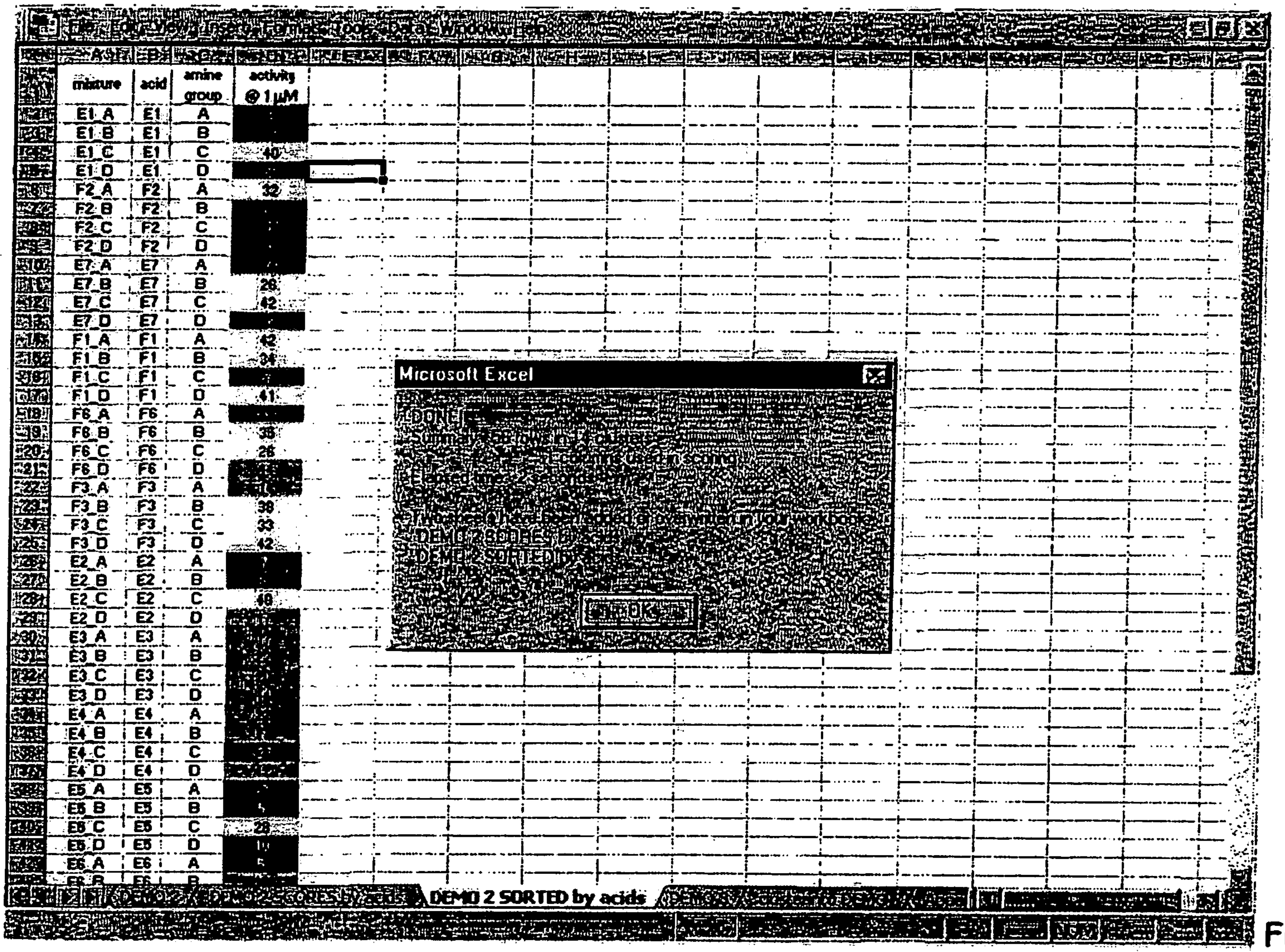
Fig. 14D



<-- Scoring of sheet "DEMO 2" using parameter set "acids"

cluster label	# of cmpds	score max. 100 (uncolored = zero)	score max. 100 (uncolored = average)
E1	4	92	92
F2	4	92	92
E7	4	83	83
F1	4	75	75
F6	4	67	67
F3	4	58	58
E2	4	50	50
E3	4	33	33
E4	4	25	25
E5	4	17	17
E6	4	17	17
F4	4	17	17
F5	4	8	8
F7	4	8	8

Fig. 15A



mixture	acid	amine group	activity @ 1 µM
E1_A	E1	A	[illegible]
E1_B	E1	B	[illegible]
E1_C	E1	C	40
E1_D	E1	D	[illegible]
F2_A	F2	A	32
F2_B	F2	B	[illegible]
F2_C	F2	C	[illegible]
F2_D	F2	D	[illegible]
E7_A	E7	A	[illegible]
E7_B	E7	B	26
E7_C	E7	C	42
E7_D	E7	D	[illegible]
F1_A	F1	A	42
F1_B	F1	B	34
F1_C	F1	C	[illegible]
F1_D	F1	D	41
F6_A	F6	A	[illegible]
F6_B	F6	B	35
F6_C	F6	C	26
F6_D	F6	D	[illegible]
F3_A	F3	A	[illegible]
F3_B	F3	B	38
F3_C	F3	C	33
F3_D	F3	D	42
E2_A	E2	A	[illegible]
E2_B	E2	B	[illegible]
E2_C	E2	C	40
E2_D	E2	D	[illegible]
E3_A	E3	A	[illegible]
E3_B	E3	B	[illegible]
E3_C	E3	C	[illegible]
E3_D	E3	D	[illegible]
E4_A	E4	A	[illegible]
E4_B	E4	B	[illegible]
E4_C	E4	C	[illegible]
E4_D	E4	D	[illegible]
E5_A	E5	A	[illegible]
E5_B	E5	B	[illegible]
E5_C	E5	C	28
E5_D	E5	D	10
E6_A	E6	A	5
E6_B	E6	B	[illegible]

Microsoft Excel

DONE!

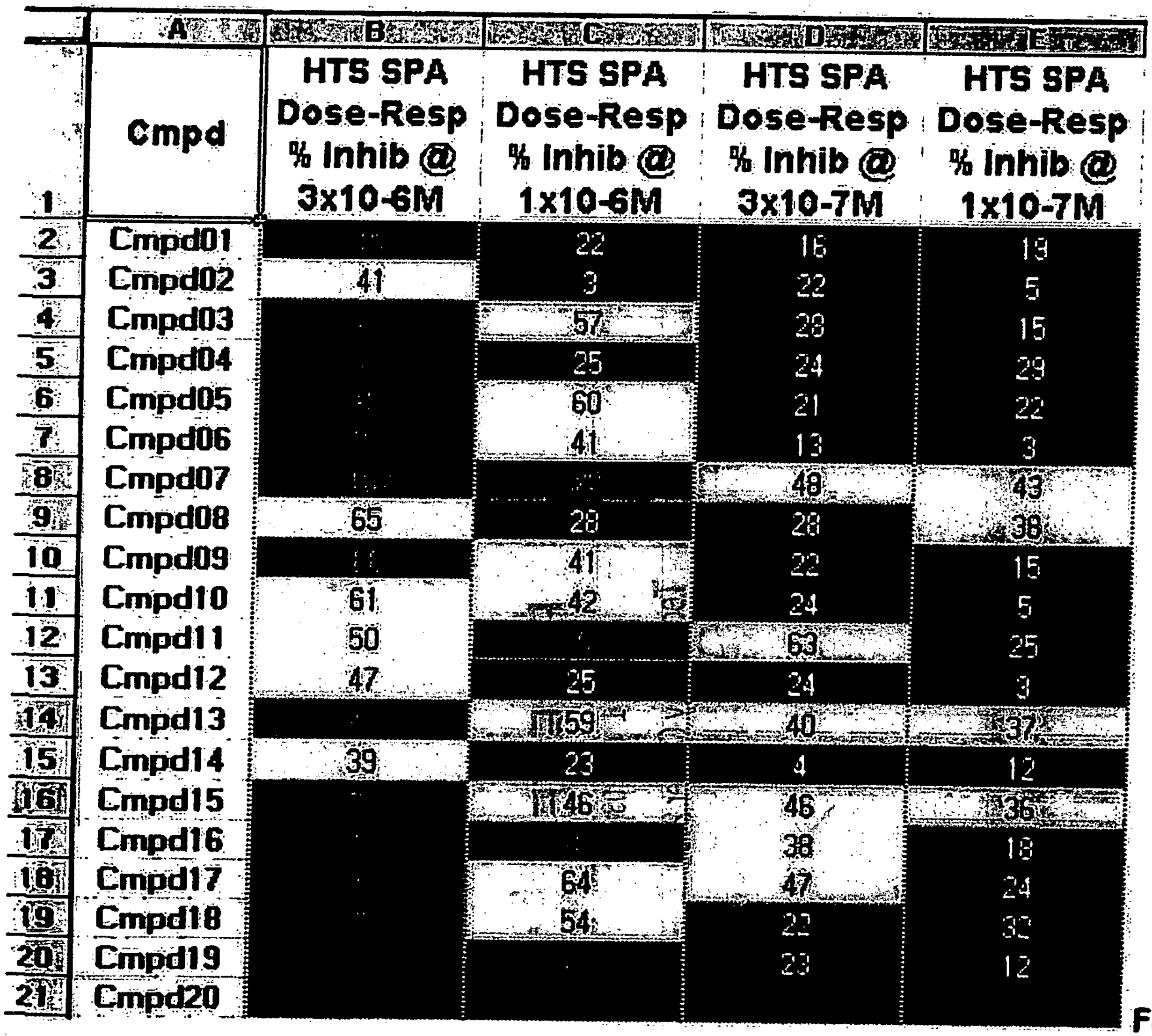
[illegible] columns used in scoring

[illegible] in your workbook:

DEMO 2 SCORES [illegible]

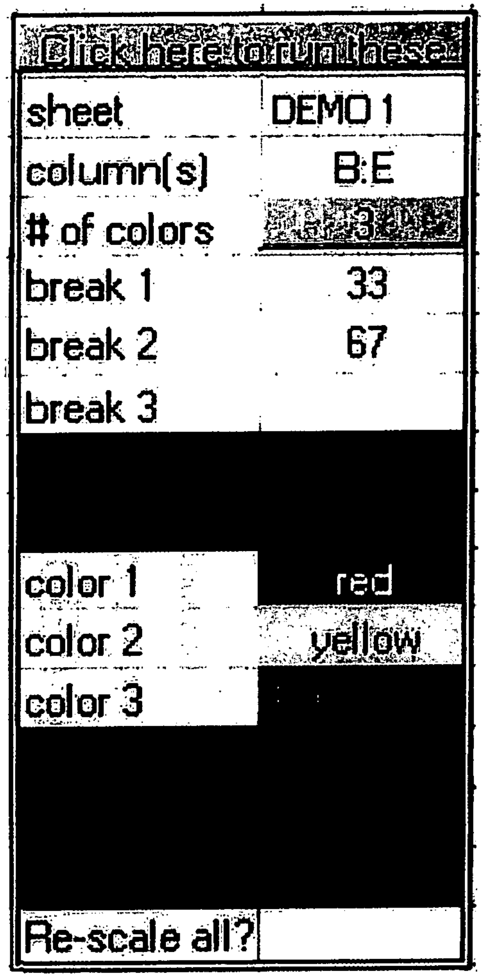
DEMO 2 SORTED [illegible]

Fig. 15B



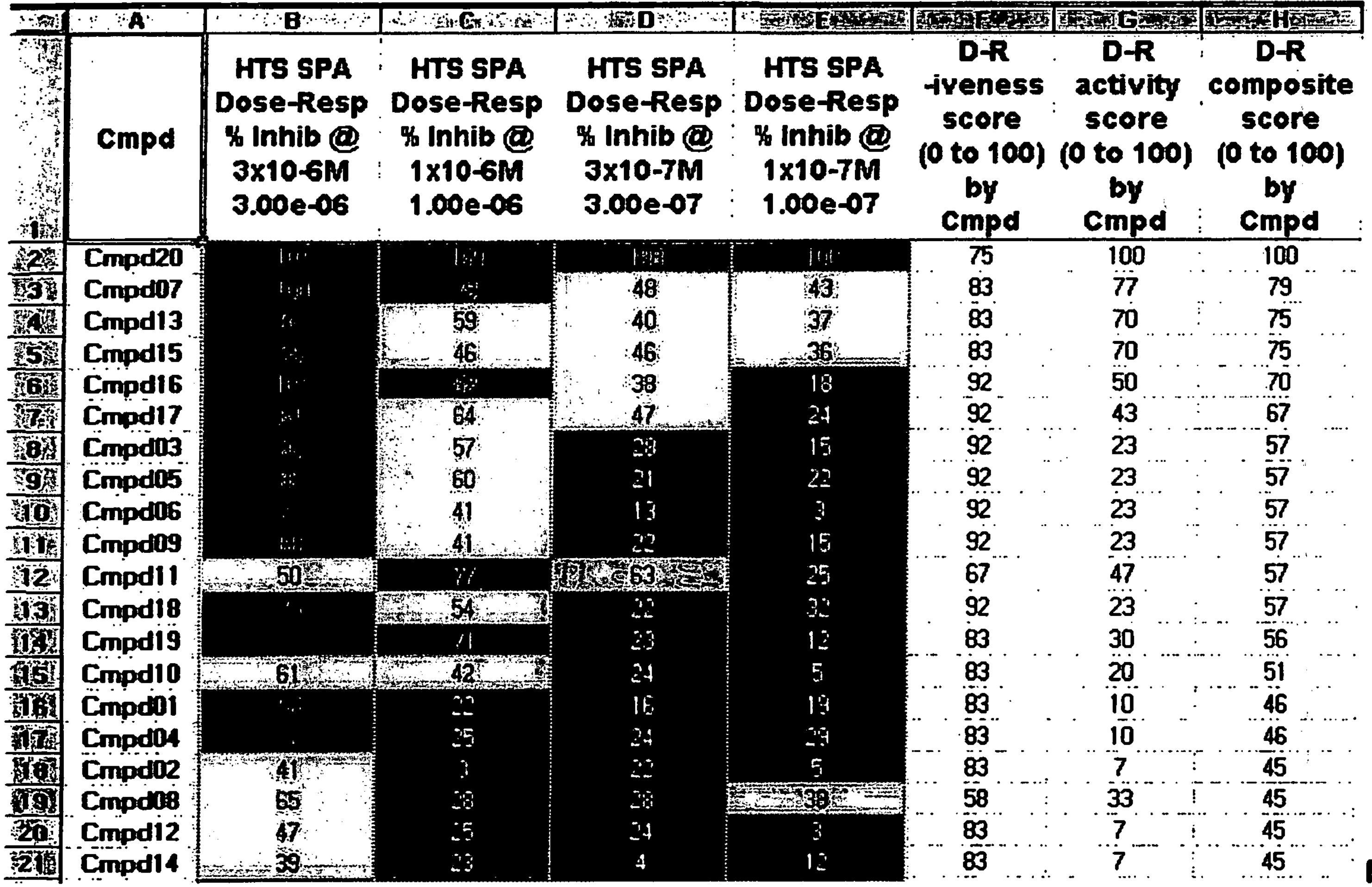
	A	B	C	D	E
1	Cmpd	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
2	Cmpd01	[illegible]	22	16	19
3	Cmpd02	41	3	22	5
4	Cmpd03		57	28	15
5	Cmpd04		25	24	29
6	Cmpd05	[illegible]	60	21	22
7	Cmpd06		41	13	3
8	Cmpd07	[illegible]	[illegible]	48	43
9	Cmpd08	65	28	28	38
10	Cmpd09	[illegible]	41	22	15
11	Cmpd10	61	42	24	5
12	Cmpd11	50	[illegible]	63	25
13	Cmpd12	47	25	24	3
14	Cmpd13		59	40	37
15	Cmpd14	39	23	4	12
16	Cmpd15		46	46	36
17	Cmpd16			38	18
18	Cmpd17		64	47	24
19	Cmpd18		54	22	32
20	Cmpd19			23	12
21	Cmpd20				

Figure 16A



sheet	DEMO 1
column(s)	B:E
# of colors	3
break 1	33
break 2	67
break 3	
color 1	red
color 2	yellow
color 3	
Re-scale all?	

Figure 16B

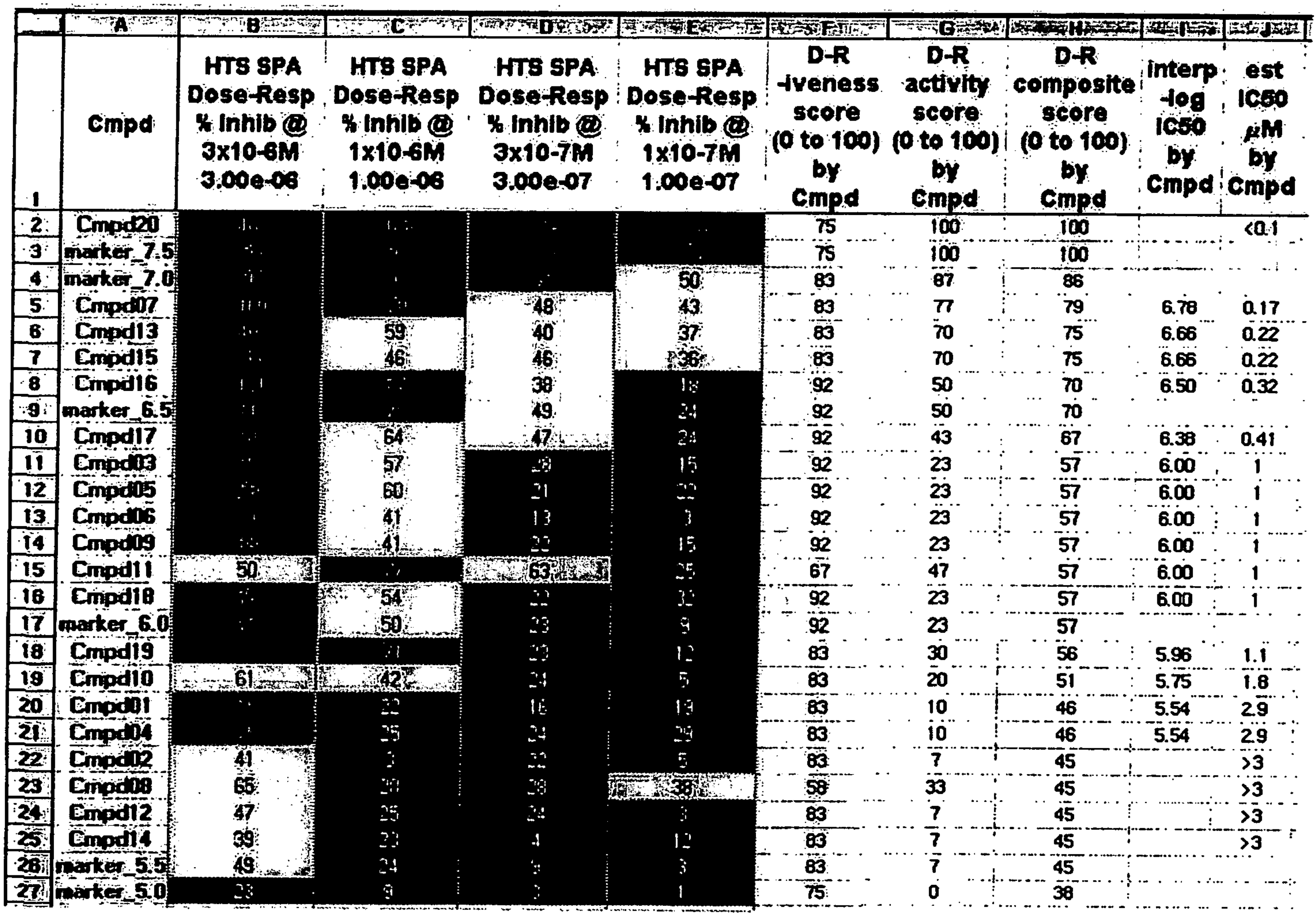


	A	B	C	D	E	F	G	H
1	Cmpd	HTS SPA Dose-Resp % Inhib @ 3x10-6M 3.00e-06	HTS SPA Dose-Resp % Inhib @ 1x10-6M 1.00e-06	HTS SPA Dose-Resp % Inhib @ 3x10-7M 3.00e-07	HTS SPA Dose-Resp % Inhib @ 1x10-7M 1.00e-07	D-R -iveness score (0 to 100) by Cmpd	D-R activity score (0 to 100) by Cmpd	D-R composite score (0 to 100) by Cmpd
2	Cmpd20	[illegible]	[illegible]	[illegible]	[illegible]	75	100	100
3	Cmpd07	[illegible]	[illegible]	48	43	83	77	79
4	Cmpd13	[illegible]	59	40	37	83	70	75
5	Cmpd15	[illegible]	46	46	36	83	70	75
6	Cmpd16	[illegible]	[illegible]	38	18	92	50	70
7	Cmpd17	[illegible]	64	47	24	92	43	67
8	Cmpd03	[illegible]	57	28	15	92	23	57
9	Cmpd05	[illegible]	60	21	22	92	23	57
10	Cmpd06	[illegible]	41	13	3	92	23	57
11	Cmpd09	[illegible]	41	22	15	92	23	57
12	Cmpd11	50	77	63	25	67	47	57
13	Cmpd18	[illegible]	54	22	32	92	23	57
14	Cmpd19	[illegible]	41	23	12	83	30	56
15	Cmpd10	61	42	24	5	83	20	51
16	Cmpd01	[illegible]	22	16	19	83	10	46
17	Cmpd04	[illegible]	35	24	29	83	10	46
18	Cmpd02	41	3	22	5	83	7	45
19	Cmpd08	65	38	28	38	58	33	45
20	Cmpd12	47	35	24	3	83	7	45
21	Cmpd14	39	23	4	12	83	7	45

Fig. 16C

	A	B	C	D	E	F	G	H
1	Cmpd	HTS SPA Dose-Resp % Inhib @ 3x10-6M 3.00e-06	HTS SPA Dose-Resp % Inhib @ 1x10-6M 1.00e-06	HTS SPA Dose-Resp % Inhib @ 3x10-7M 3.00e-07	HTS SPA Dose-Resp % Inhib @ 1x10-7M 1.00e-07	D-R -iveness score (0 to 100) by Cmpd	D-R activity score (0 to 100) by Cmpd	D-R composite score (0 to 100) by Cmpd
22	marker_7.5	[illegible]	[illegible]	[illegible]	[illegible]	75	100	100
23	marker_7.0	[illegible]	[illegible]	[illegible]	50	83	87	86
24	marker_6.5	[illegible]	[illegible]	49	24	92	50	70
25	marker_6.0	[illegible]	50	23	9	92	23	57
26	marker_5.5	49	24	9	3	83	7	45
27	marker_5.0	23	9	3	1	75	0	38

Figure 16D



	A	B	C	D	E	F	G	H	I	J
1	Cmpd	HTS SPA Dose-Resp % Inhib @ 3x10-6M 3.00e-06	HTS SPA Dose-Resp % Inhib @ 1x10-6M 1.00e-06	HTS SPA Dose-Resp % Inhib @ 3x10-7M 3.00e-07	HTS SPA Dose-Resp % Inhib @ 1x10-7M 1.00e-07	D-R -iveness score (0 to 100) by Cmpd	D-R activity score (0 to 100) by Cmpd	D-R composite score (0 to 100) by Cmpd	interp -log IC50 by Cmpd	est IC50 µM by Cmpd
2	Cmpd20	[illegible]	[illegible]	[illegible]	[illegible]	75	100	100		<0.1
3	marker_7.5	[illegible]	[illegible]	[illegible]	[illegible]	75	100	100		
4	marker_7.0	[illegible]	[illegible]	[illegible]	50	83	87	86		
5	Cmpd07	[illegible]	[illegible]	48	43	83	77	79	6.78	0.17
6	Cmpd13	[illegible]	59	40	37	83	70	75	6.66	0.22
7	Cmpd15	[illegible]	46	46	36	83	70	75	6.66	0.22
8	Cmpd16	[illegible]	[illegible]	38	18	92	50	70	6.50	0.32
9	marker_6.5	[illegible]	[illegible]	49	24	92	50	70		
10	Cmpd17	[illegible]	64	47	24	92	43	67	6.38	0.41
11	Cmpd03	[illegible]	57	28	15	92	23	57	6.00	1
12	Cmpd05	[illegible]	60	21	22	92	23	57	6.00	1
13	Cmpd06	[illegible]	41	13	3	92	23	57	6.00	1
14	Cmpd09	[illegible]	41	22	15	92	23	57	6.00	1
15	Cmpd11	50	[illegible]	63	25	67	47	57	6.00	1
16	Cmpd18	[illegible]	54	22	32	92	23	57	6.00	1
17	marker_6.0	[illegible]	50	23	9	92	23	57		
18	Cmpd19	[illegible]	21	23	12	83	30	56	5.96	1.1
19	Cmpd10	61	42	24	5	83	20	51	5.75	1.8
20	Cmpd01	[illegible]	22	16	19	83	10	46	5.54	2.9
21	Cmpd04	[illegible]	25	24	29	83	10	46	5.54	2.9
22	Cmpd02	41	3	22	5	83	7	45		>3
23	Cmpd08	66	20	28	38	58	33	45		>3
24	Cmpd12	47	25	24	3	83	7	45		>3
25	Cmpd14	39	23	4	12	83	7	45		>3
26	marker_5.5	49	24	9	3	83	7	45		
27	marker_5.0	28	9	3	1	75	0	38		

Figure 16E

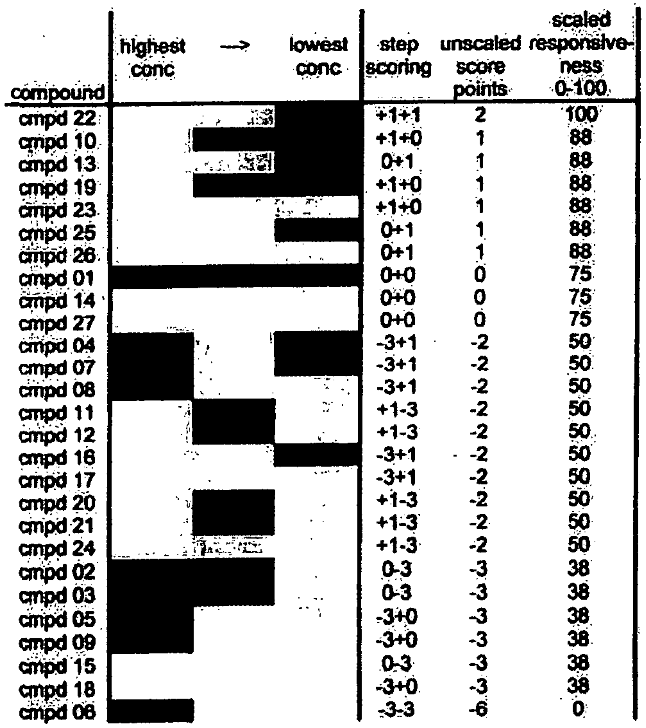
Fig. 16F

The complete data set for 3 points and 3 colors, in systematic order.

	percent inhibition			data group number			data group color		
compound	highest conc	--->	lowest conc	highest conc	--->	lowest conc	highest conc	--->	lowest conc
cmpd 01	2	29	22	1	1	1	■	■	■
cmpd 02	16	10	38	1	1	2	■	■	□
cmpd 03	31	26	79	1	1	3	■	■	□
cmpd 04	21	46	25	1	2	1	■	□	■
cmpd 05	30	53	61	1	2	2	■	□	□
cmpd 06	17	37	70	1	2	3	■	□	□
cmpd 07	26	90	17	1	3	1	■	□	■
cmpd 08	10	90	38	1	3	2	■	□	□
cmpd 09	32	72	94	1	3	3	■	□	□
cmpd 10	34	17	15	2	1	1	□	■	■
cmpd 11	51	8	42	2	1	2	□	■	□
cmpd 12	56	3	69	2	1	3	□	■	□
cmpd 13	33	39	14	2	2	1	□	□	■
cmpd 14	53	52	55	2	2	2	□	□	□
cmpd 15	51	62	87	2	2	3	□	□	□
cmpd 16	65	82	6	2	3	1	□	□	■
cmpd 17	43	71	41	2	3	2	□	□	□
cmpd 18	65	99	77	2	3	3	□	□	□
cmpd 19	67	11	9	3	1	1	□	■	■
cmpd 20	87	5	66	3	1	2	□	■	□
cmpd 21	77	8	70	3	1	3	□	■	□
cmpd 22	78	36	0	3	2	1	□	□	■
cmpd 23	85	40	63	3	2	2	□	□	□
cmpd 24	83	57	88	3	2	3	□	□	□
cmpd 25	73	88	15	3	3	1	□	□	■
cmpd 26	69	85	35	3	3	2	□	□	□
cmpd 27	79	68	91	3	3	3	□	□	□

Fig. 16G

The complete data set for 3 points and 3 colors, sorted by decreasing dose-responsiveness



compound	highest conc	--->	lowest conc	step scoring	unscaled score points	scaled responsive-ness 0-100
cmpd 22			■	+1+1	2	100
cmpd 10		■	■	+1+0	1	88
cmpd 13			■	0+1	1	88
cmpd 19		■	■	+1+0	1	88
cmpd 23				+1+0	1	88
cmpd 25			■	0+1	1	88
cmpd 26				0+1	1	88
cmpd 01	■	■	■	0+0	0	75
cmpd 14				0+0	0	75
cmpd 27				0+0	0	75
cmpd 04	■		■	-3+1	-2	50
cmpd 07	■		■	-3+1	-2	50
cmpd 08	■			-3+1	-2	50
cmpd 11		■		+1-3	-2	50
cmpd 12		■		+1-3	-2	50
cmpd 16			■	-3+1	-2	50
cmpd 17				-3+1	-2	50
cmpd 20		■		+1-3	-2	50
cmpd 21		■		+1-3	-2	50
cmpd 24				+1-3	-2	50
cmpd 02	■	■		0-3	-3	38
cmpd 03	■	■		0-3	-3	38
cmpd 05	■			-3+0	-3	38
cmpd 09	■			-3+0	-3	38
cmpd 15				0-3	-3	38
cmpd 18				-3+0	-3	38
cmpd 06	■			-3-3	-6	0

Fig. 16H

The complete set of data for 3 points and 3 colors, sorted by decreasing overall activity.

	data group number			data group color					
compound	highest conc	—>	lowest conc	highest conc	—>	lowest conc	activity scoring	unscaled activity points	scaled activity 0-100
cmpd 27	3	3	3	□	□	□	1(3)+2(3)+3(3)	18	100
cmpd 18	2	3	3	□	□	□	1(2)+2(3)+3(3)	17	92
cmpd 24	3	2	3	□	□	□	1(3)+2(2)+3(3)	16	83
cmpd 09	1	3	3	■	□	□	1(1)+2(3)+3(3)	16	83
cmpd 26	3	3	2	□	□	□	1(3)+2(3)+3(2)	15	75
cmpd 15	2	2	3	□	□	□	1(2)+2(2)+3(3)	15	75
cmpd 17	2	3	2	□	□	□	1(2)+2(3)+3(2)	14	67
cmpd 21	3	1	3	□	■	□	1(3)+2(1)+3(3)	14	67
cmpd 06	1	2	3	■	□	□	1(1)+2(2)+3(3)	14	67
cmpd 23	3	2	2	□	□	□	1(3)+2(2)+3(2)	13	58
cmpd 08	1	3	2	■	□	□	1(1)+2(3)+3(2)	13	58
cmpd 12	2	1	3	□	■	□	1(2)+2(1)+3(3)	13	58
cmpd 25	3	3	1	□	□	■	1(3)+2(3)+3(1)	12	50
cmpd 14	2	2	2	□	□	□	1(2)+2(2)+3(2)	12	50
cmpd 03	1	1	3	■	■	□	1(1)+2(1)+3(3)	12	50
cmpd 16	2	3	1	□	□	■	1(2)+2(3)+3(1)	11	42
cmpd 20	3	1	2	□	■	□	1(3)+2(1)+3(2)	11	42
cmpd 05	1	2	2	■	□	□	1(1)+2(2)+3(2)	11	42
cmpd 22	3	2	1	□	□	■	1(3)+2(2)+3(1)	10	33
cmpd 07	1	3	1	■	□	■	1(1)+2(3)+3(1)	10	33
cmpd 11	2	1	2	□	■	▨	1(2)+2(1)+3(2)	10	33
cmpd 13	2	2	1	□	▨	■	1(2)+2(2)+3(1)	9	25
cmpd 02	1	1	2	■	■	▨	1(1)+2(1)+3(2)	9	25
cmpd 19	3	1	1	□	■	■	1(3)+2(1)+3(1)	8	17
cmpd 04	1	2	1	■	▨	■	1(1)+2(2)+3(1)	8	17
cmpd 10	2	1	1	□	■	■	1(2)+2(1)+3(1)	7	8
cmpd 01	1	1	1	■	■	■	1(1)+2(1)+3(1)	6	0

Fig. 16I

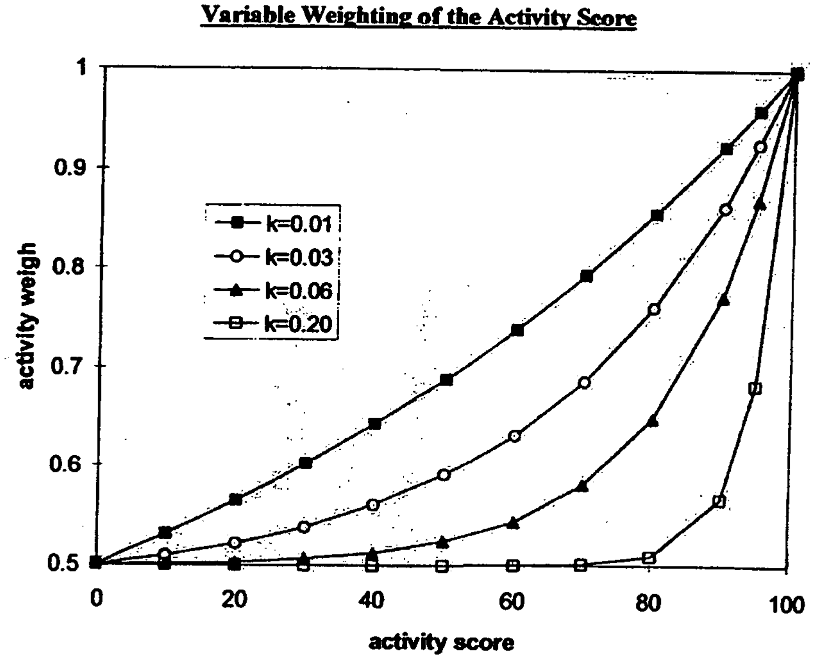
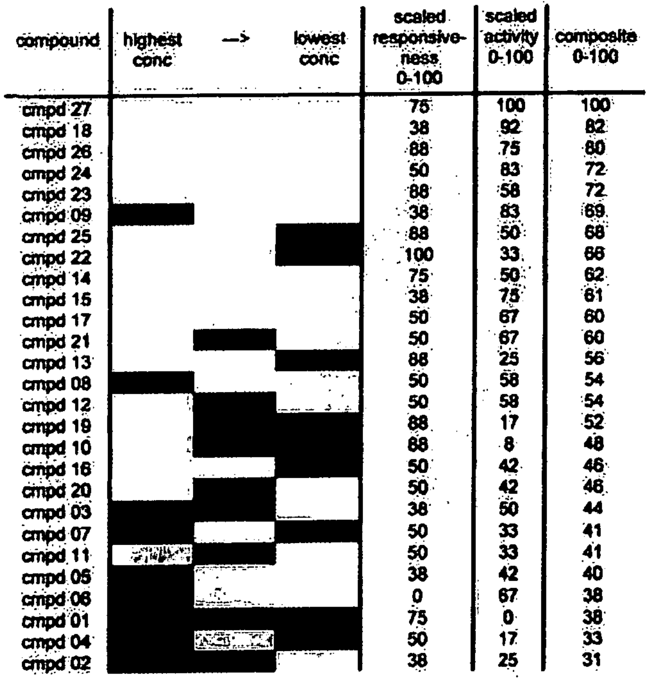

Variable Weighting of the Activity Score
activity weigh
1
0.9
0.8
0.7
0.6
0.5
0
20
40
60
80
100
activity score
k=0.01
k=0.03
k=0.06
k=0.20

Fig. 16J

The complete set of data for 3 points and 3 colors, sorted by decreasing composite score.



compound	highest conc	—>	lowest conc	scaled responsive-ness 0-100	scaled activity 0-100	composite 0-100
cmpd 27	□	□	□	75	100	100
cmpd 18	□	□	□	38	92	82
cmpd 26	□	□	□	88	75	80
cmpd 24	□	□	□	50	83	72
cmpd 23	□	□	□	88	58	72
cmpd 09	■	□	□	38	83	69
cmpd 25	□	□	■	88	50	68
cmpd 22	□	□	■	100	33	66
cmpd 14	□	□	□	75	50	62
cmpd 15	□	□	□	38	75	61
cmpd 17	□	□	□	50	67	60
cmpd 21	□	■	□	50	67	60
cmpd 13	□	□	■	88	25	56
cmpd 08	■	□	□	50	58	54
cmpd 12	□	■	□	50	58	54
cmpd 19	□	■	■	88	17	52
cmpd 10	□	■	■	88	8	48
cmpd 16	□	□	■	50	42	46
cmpd 20	□	■	□	50	42	46
cmpd 03	■	■	□	38	50	44
cmpd 07	■	□	■	50	33	41
cmpd 11	▨	■	□	50	33	41
cmpd 05	■	□	□	38	42	40
cmpd 06	■	□	□	0	67	38
cmpd 01	■	■	■	75	0	38
cmpd 04	■	▨	■	50	17	33
cmpd 02	■	■	□	38	25	31

Fig. 16K

Quality of Ranking when Noise = 10 Inhibition Percentage Points

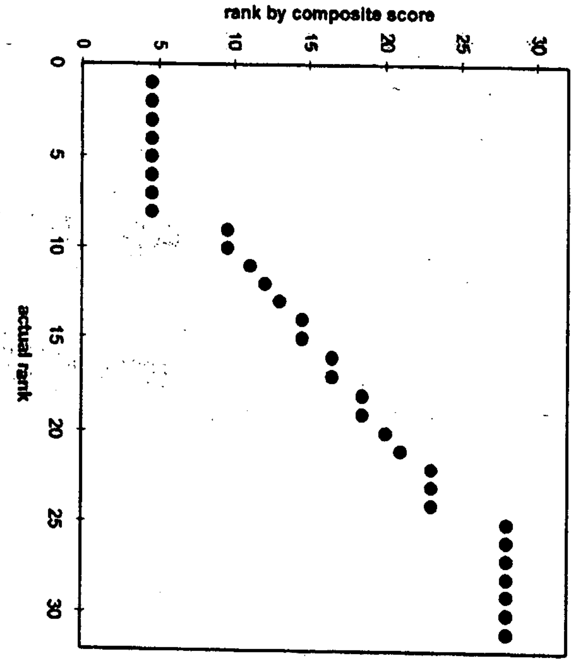


Fig. 16L

Quality of Ranking when Noise = 30 Inhibition Percentage Points

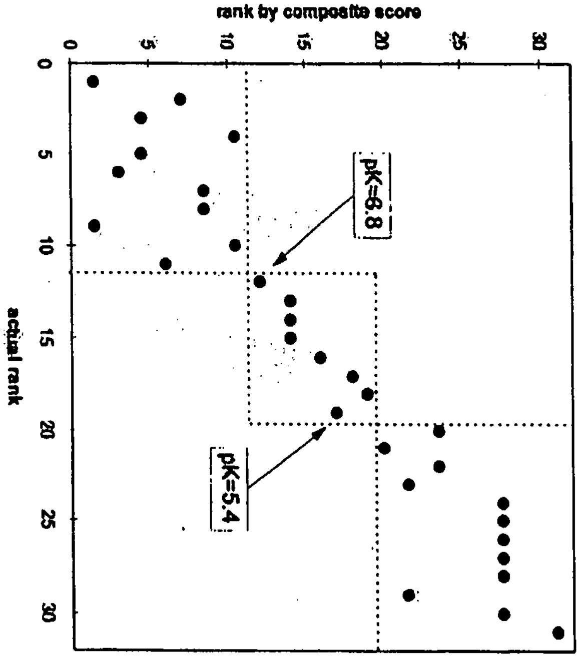


Fig. 16M

Quantitative Estimation of Potencies by Calibration Marker Compounds

compound	% Inhib @ 3.00e-06	% Inhib @ 1.00e-06	% Inhib @ 3.00e-07	% Inhib @ 1.00e-07	D-R composite score	interp -log IC50	est IC50 µM
M353876	100	102	83	75	79		<0.1
marker_7.5	**99**	**97**	**90**	**76**	**79**		
M221211	110	91	69	39	76	7.00	0.10
M371585	108	102	63	27	76	7.00	0.10
marker_7.0	**97**	**91**	**75**	50	**76**		
M345077	102	87	92	87	75	6.97	0.11
M371796	91	78	76	33	73	6.90	0.13
M143629	100	79	48	43	69	6.77	0.17
M371890	101	72	42	29	69	6.77	0.17
M371891	92	69	55	49	69	6.77	0.17
M309032	105	62	62	[illegible]	67	6.70	0.20
M198289	101	82	38	[illegible]	66	6.67	0.22
M224602	97	79	43	[illegible]	66	6.67	0.22
M318671	93	63	42	[illegible]	66	6.67	0.22
M273373	95	93	52	[illegible]	65	6.63	0.23
M371336	78	70	44	27	62	6.53	0.29
M371825	61	64	60	26	62	6.53	0.29
M181250	99	46	46	36	61	6.50	0.32
M338331	87	73	29	[illegible]	61	6.50	0.32
marker_6.5	**90**	**76**	**49**	24	**61**		
M143630	65	28	28	38	60	6.44	0.36

Fig. 16N

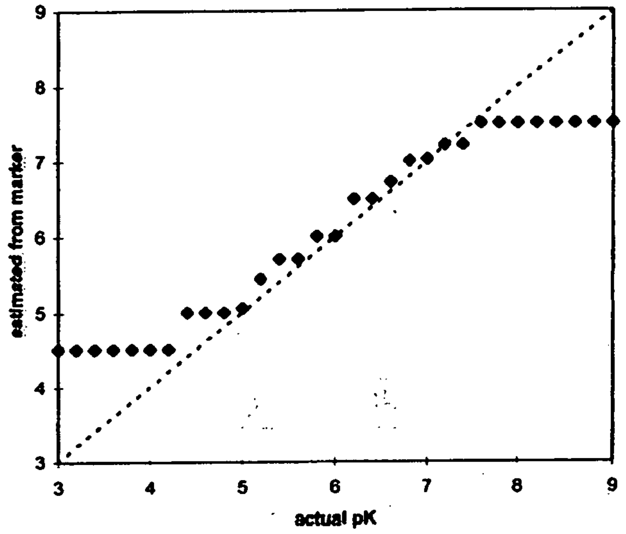

Quality of Estimation when Noise = 10 Inhibition Percentage Points
estimated from marker
3
4
5
6
7
8
9
actual pK
3
4
5
6
7
8
9

Fig. 16P

Quality of Estimation when Noise = 30 Inhibition Percentage Points

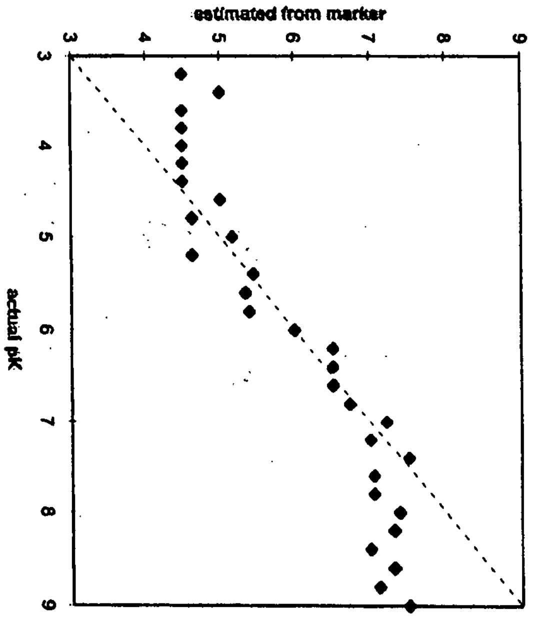
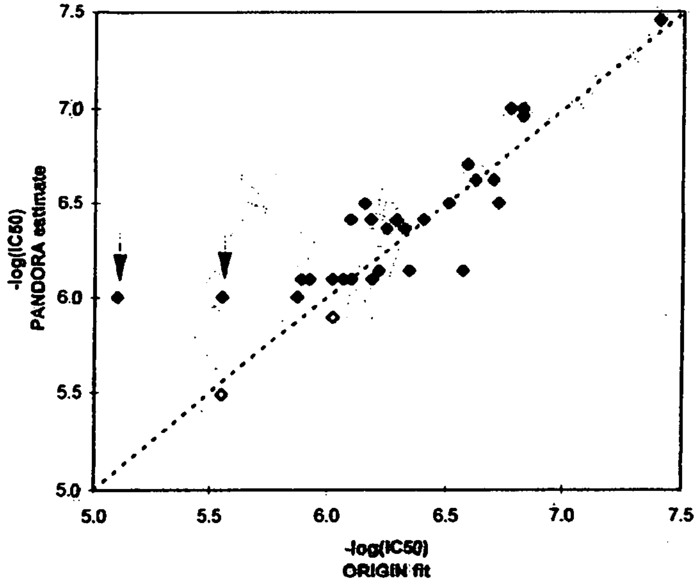


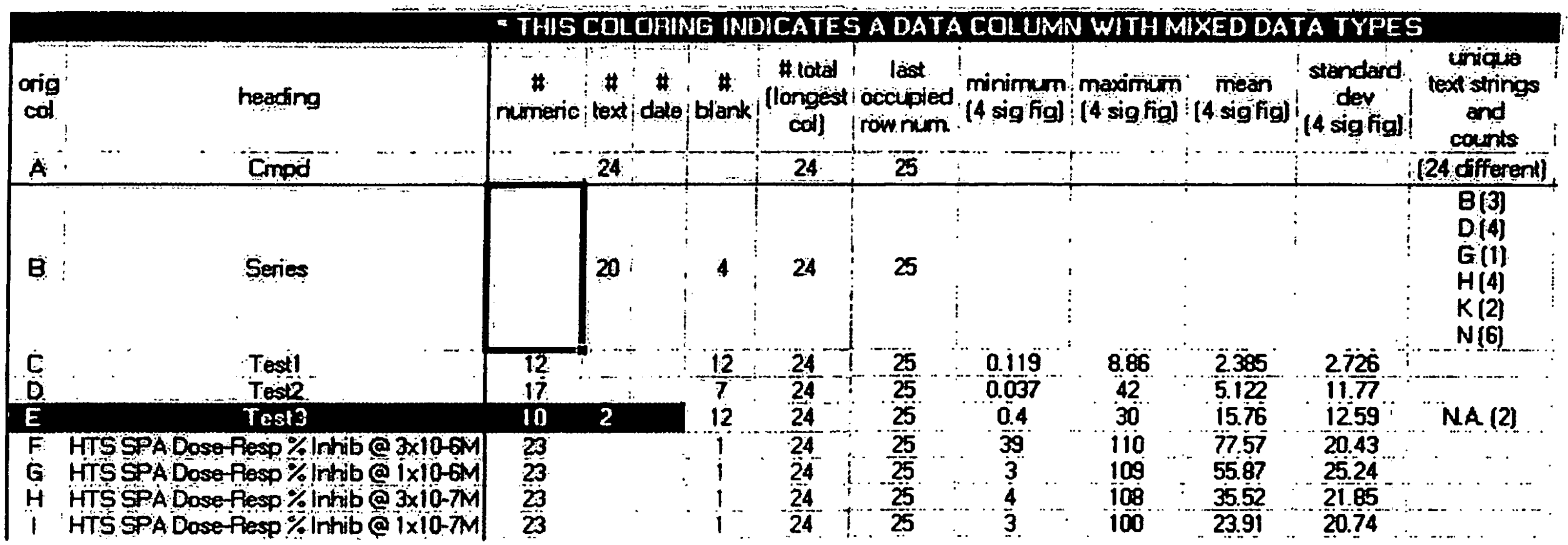
Fig. 16Q

Comparison of Curve Fitting to Marker Calibration
for T-cell Proliferation Data



	A	B	C	D	E	F	G	H	I
1	Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
2	Cmpd01	N		29	30				
3	Cmpd02	N		42	5.5	41	3	22	5
4	Cmpd03	G		2.61	11	83	57	28	15
5	Cmpd04	N			30	70	25	24	29
6	Cmpd05	N		1.8	9.2	89	60	21	22
7	Cmpd06	D	8.86	6.5	3.7	71	41	13	3
8	Cmpd07	D	3.11	0.037	7.8	100	79	48	43
9	Cmpd08	D		0.089	N.A.	65	28	28	38
10	Cmpd09	D	0.119			68	41	22	15
11	Cmpd10	N	0.233			61	42	24	5
12	Cmpd11	N	4.31			50	77	63	25
13	Cmpd12	H	1.3	0.24		47	25	24	3
14	Cmpd13	H	1.17	0.194	30	81	59	40	37
15	Cmpd14	H	0.26	0.41		39	23	4	12
16	Cmpd15	H	0.369	0.148		99	46	46	36
17	Cmpd16			0.87	30	101	82	38	18
18	Cmpd17	K		0.223	N.A.	81	64	47	24
19	Cmpd18		5.27			79	54	22	32
20	Cmpd19		0.134			71	71	23	12
21	Cmpd20			0.317		101	109	108	100
22	Cmpd21	K		2.21		87	70	31	13
23	Cmpd22	B		0.15		94	77	36	12
24	Cmpd23	B				96	61	36	12
25	Cmpd24	B	3.487	0.27	0.4	110	91	69	39

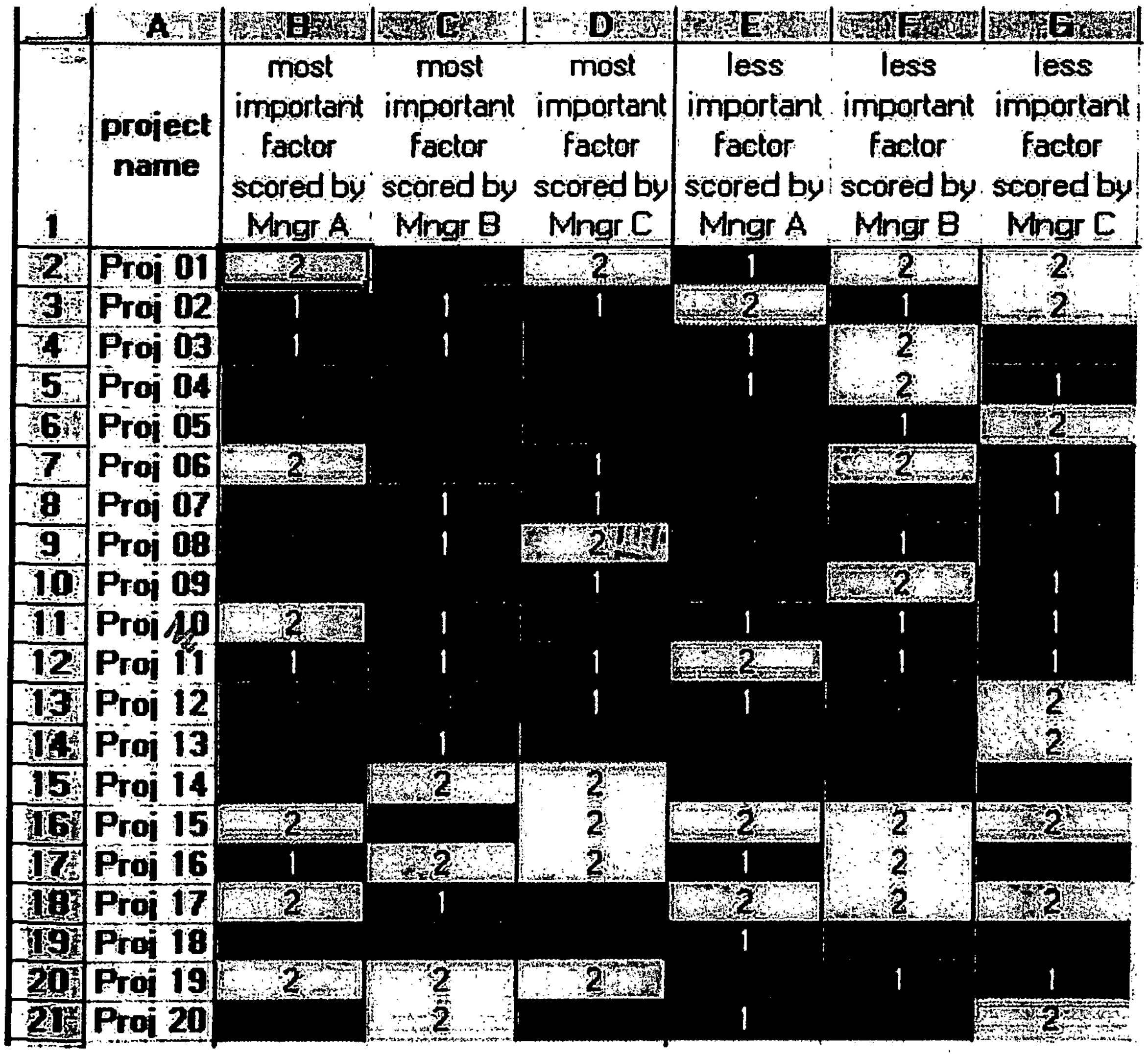
Figure 17A



* THIS COLORING INDICATES A DATA COLUMN WITH MIXED DATA TYPES

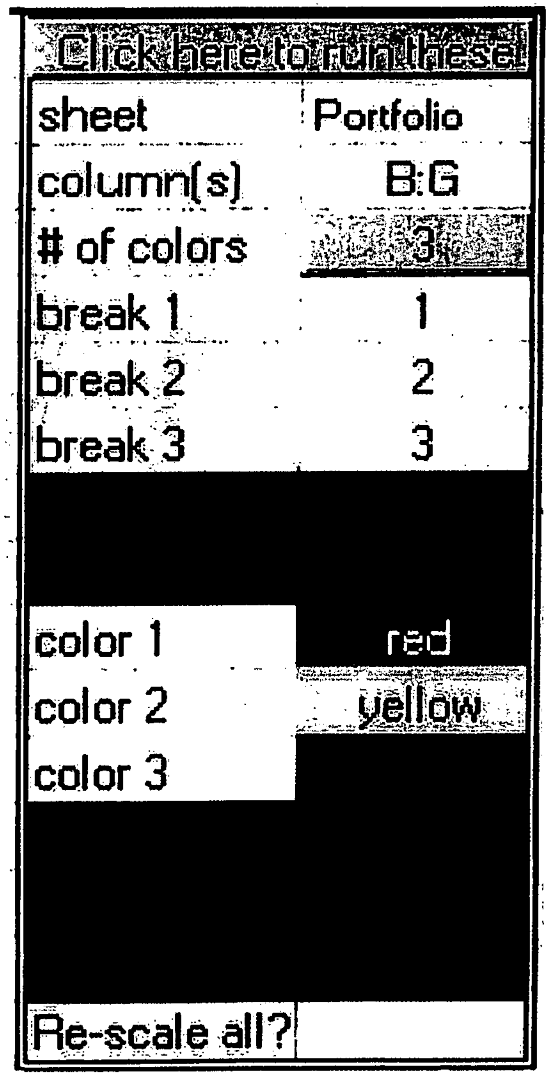
orig col	heading	# numeric	# text	# date	# blank	# total (longest col)	last occupied row num.	minimum (4 sig fig)	maximum (4 sig fig)	mean (4 sig fig)	standard dev (4 sig fig)	unique text strings and counts
A	Cmpd		24			24	25					(24 different)
B	Series		20		4	24	25					B (3) D (4) G (1) H (4) K (2) N (6)
C	Test1	12			12	24	25	0.119	8.86	2.385	2.726	
D	Test2	17			7	24	25	0.037	42	5.122	11.77	
E	Test3	10	2		12	24	25	0.4	30	15.76	12.59	N.A. (2)
F	HTS SPA Dose-Resp % Inhib @ 3x10-6M	23			1	24	25	39	110	77.57	20.43	
G	HTS SPA Dose-Resp % Inhib @ 1x10-6M	23			1	24	25	3	109	55.87	25.24	
H	HTS SPA Dose-Resp % Inhib @ 3x10-7M	23			1	24	25	4	108	35.52	21.85	
I	HTS SPA Dose-Resp % Inhib @ 1x10-7M	23			1	24	25	3	100	23.91	20.74	

Figure 17B



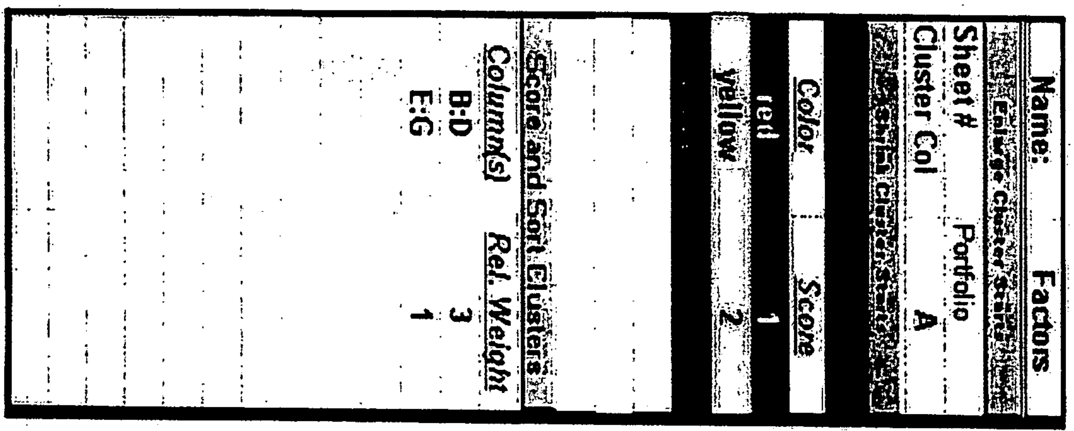
	A	B	C	D	E	F	G
1	project name	most important factor scored by Mngr A	most important factor scored by Mngr B	most important factor scored by Mngr C	less important factor scored by Mngr A	less important factor scored by Mngr B	less important factor scored by Mngr C
2	Proj 01	2		2	1	2	2
3	Proj 02	1	1	1	2	1	2
4	Proj 03	1	1		1	2	
5	Proj 04				1	2	1
6	Proj 05					1	2
7	Proj 06	2		1		2	1
8	Proj 07		1	1			1
9	Proj 08		1	2		1	
10	Proj 09			1		2	1
11	Proj 10	2	1		1	1	1
12	Proj 11	1	1	1	2	1	1
13	Proj 12			1	1		2
14	Proj 13		1				2
15	Proj 14		2	2			
16	Proj 15	2		2	2	2	2
17	Proj 16	1	2	2	1	2	
18	Proj 17	2	1		2	2	2
19	Proj 18				1		
20	Proj 19	2	2	2		1	1
21	Proj 20		2		1		2

Figure 18A



sheet	Portfolio
column(s)	B:G
# of colors	3
break 1	1
break 2	2
break 3	3
color 1	red
color 2	yellow
color 3	
Re-scale all?	

Figure 18B

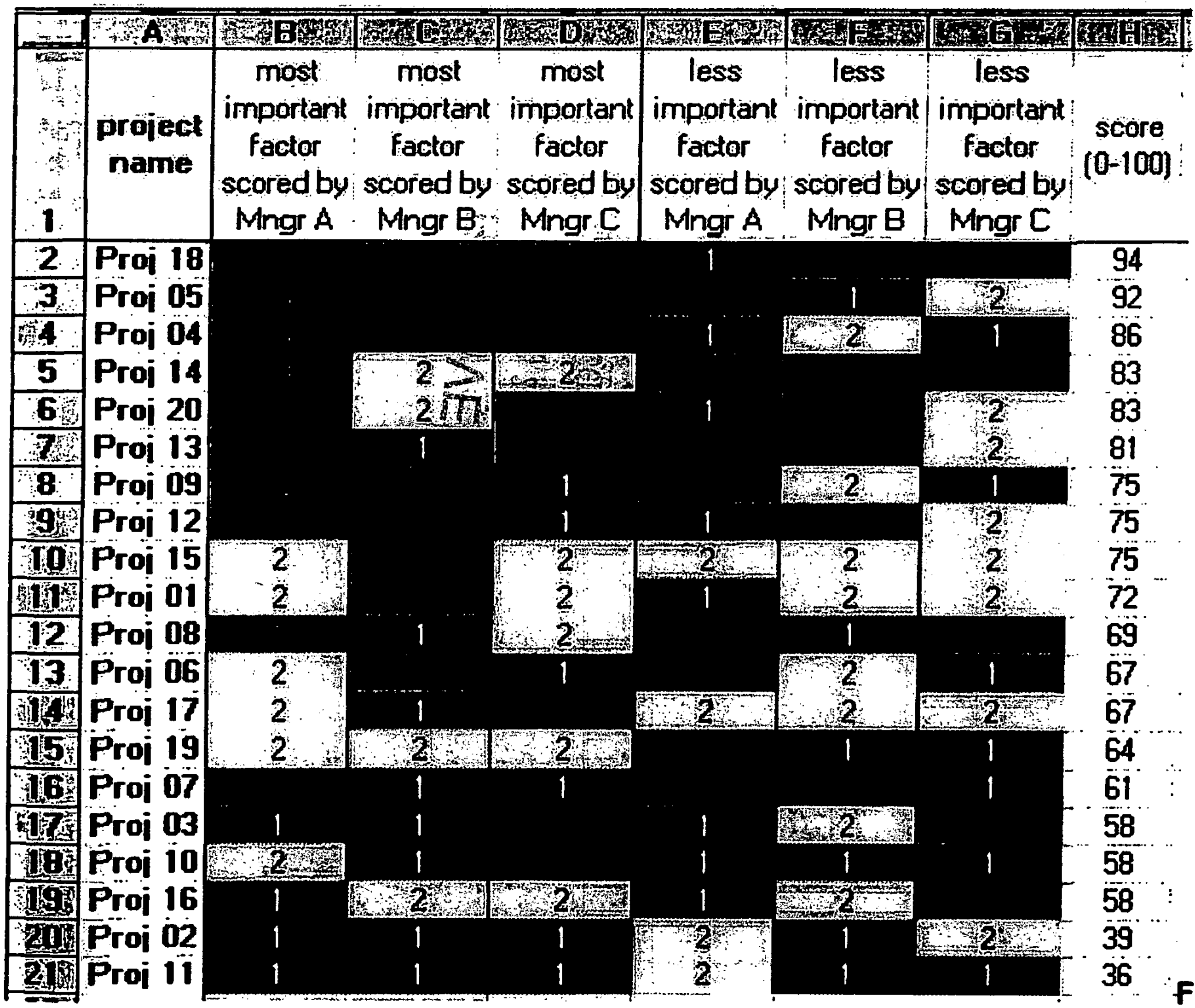


Name:	Factors
Enlarge Cluster Starts	
Sheet #	Portfolio
Cluster Col	A
[illegible] Cluster Starts	
Color	*Score*
red	1
yellow	2

Score and Sort Clusters

Column(s)	*Rel. Weight*
B:D	3
E:G	1

Figure 18C

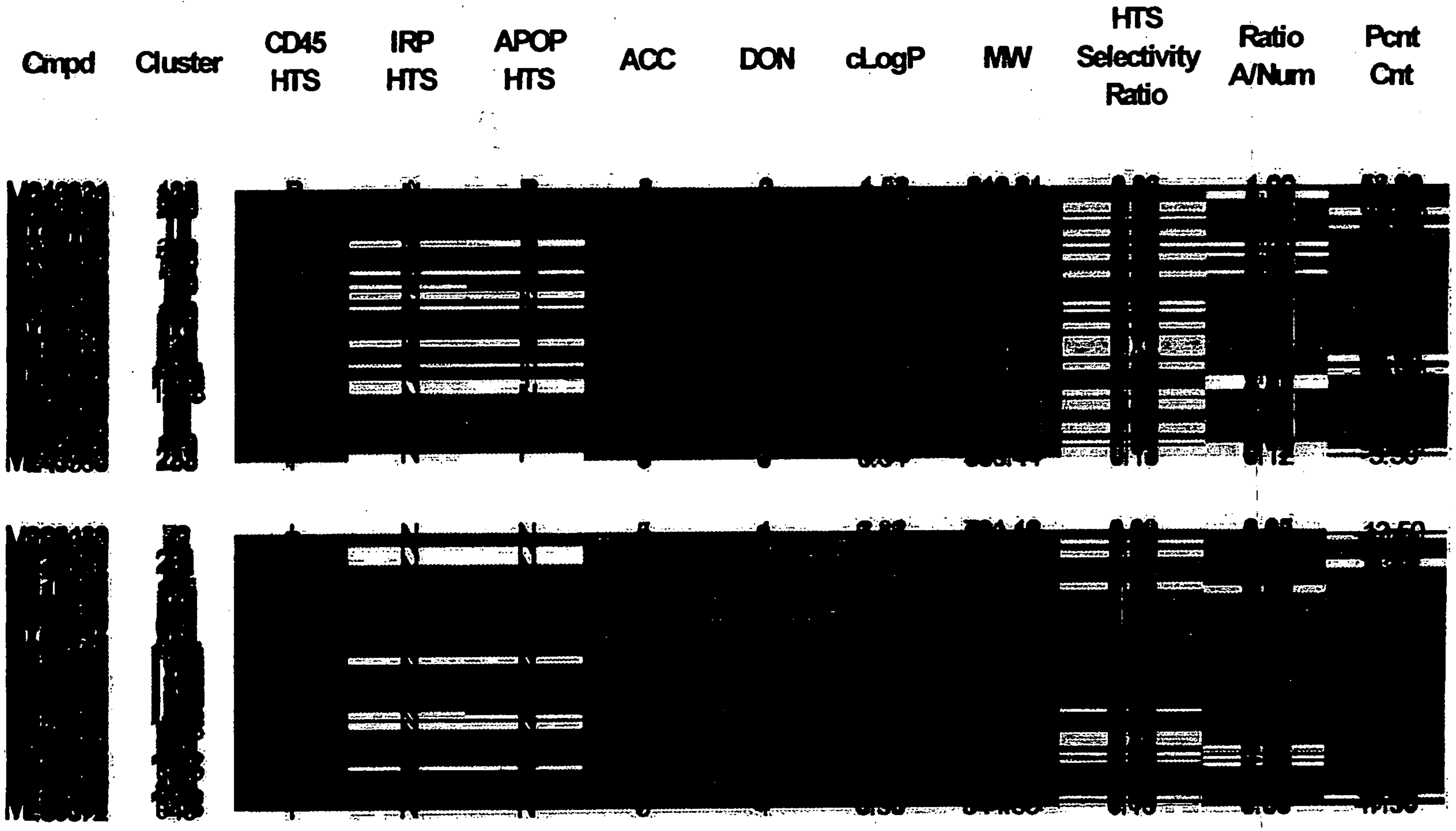


	A	B	C	D	E	F	G	H
1	project name	most important factor scored by Mngr A	most important factor scored by Mngr B	most important factor scored by Mngr C	less important factor scored by Mngr A	less important factor scored by Mngr B	less important factor scored by Mngr C	score (0-100)
2	Proj 18				1			94
3	Proj 05					1	2	92
4	Proj 04				1	2	1	86
5	Proj 14		2	2				83
6	Proj 20		2		1		2	83
7	Proj 13		1				2	81
8	Proj 09			1		2	1	75
9	Proj 12			1	1		2	75
10	Proj 15	2		2	2	2	2	75
11	Proj 01	2		2	1	2	2	72
12	Proj 08		1	2		1		69
13	Proj 06	2		1		2	1	67
14	Proj 17	2	1		2	2	2	67
15	Proj 19	2	2	2		1	1	64
16	Proj 07		1	1			1	61
17	Proj 03	1	1		1	2		58
18	Proj 10	2	1		1	1	1	58
19	Proj 16	1	2	2	1	2		58
20	Proj 02	1	1	1	2	1	2	39
21	Proj 11	1	1	1	2	1	1	36

Figure 18D

Fig. 19

Drug Candidate Compounds;
Scored, Sorted, and Vertically Compressed



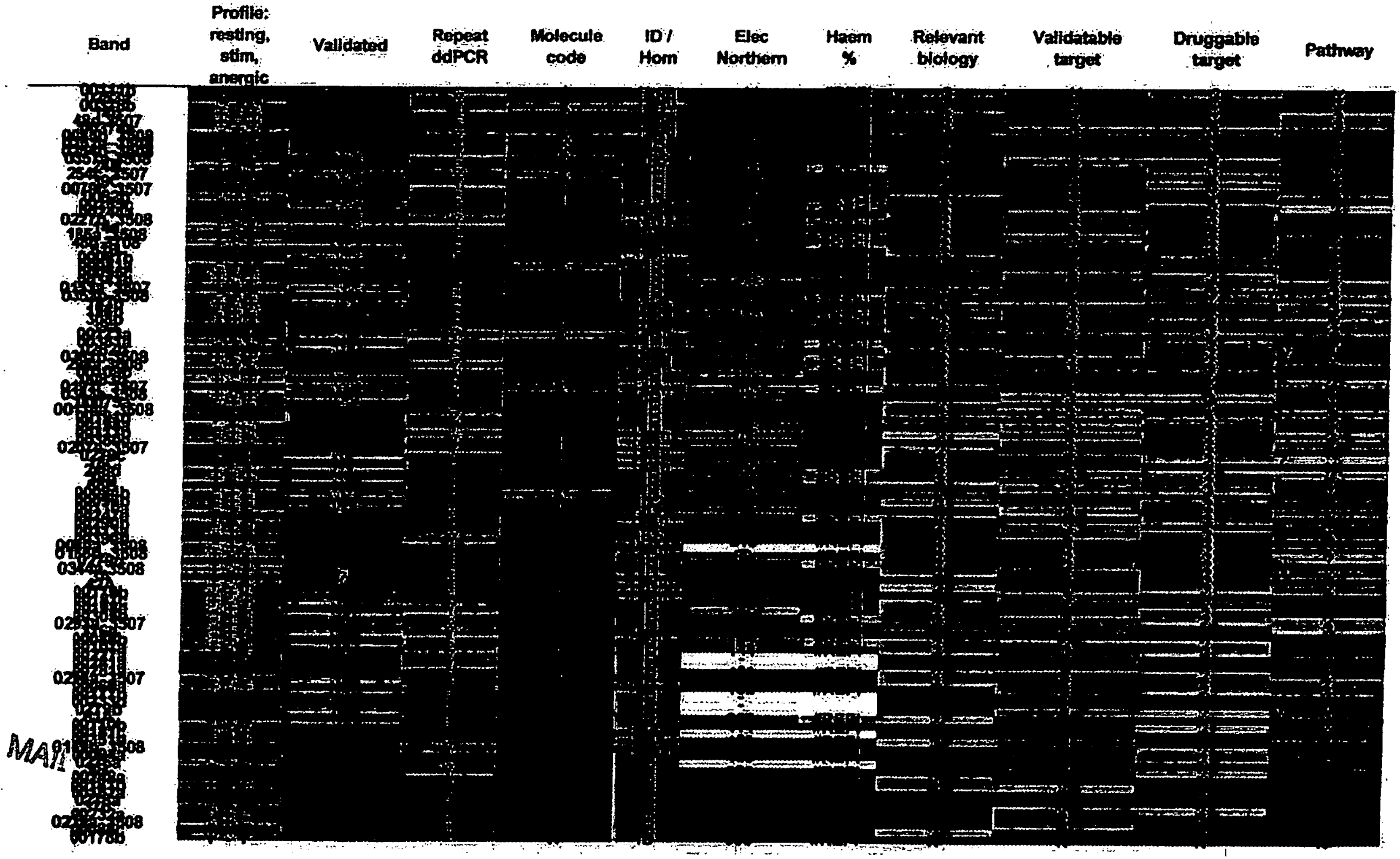
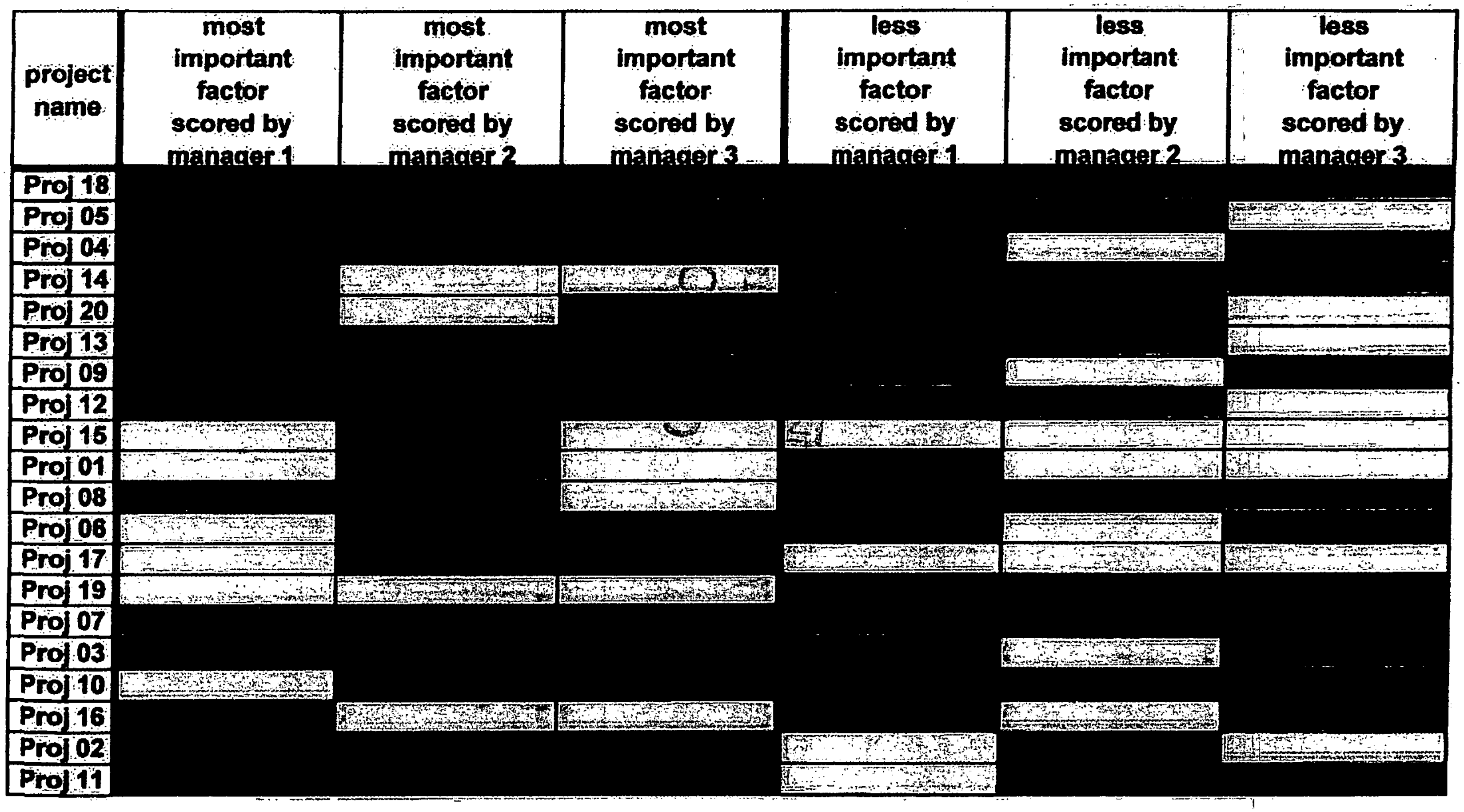


Fig. 20 Target Protein Candidates



project name	most important factor scored by manager 1	most important factor scored by manager 2	most important factor scored by manager 3	less important factor scored by manager 1	less important factor scored by manager 2	less important factor scored by manager 3
Proj 18	■	■	■	■	■	■
Proj 05	■	■	■	■	■	□
Proj 04	■	■	■	■	□	■
Proj 14	■	□	□	■	■	■
Proj 20	■	□	■	■	■	□
Proj 13	■	■	■	■	■	□
Proj 09	■	■	■	■	□	■
Proj 12	■	■	■	■	■	□
Proj 15	□	■	□	□	□	□
Proj 01	□	■	□	■	□	□
Proj 08	■	■	□	■	■	■
Proj 06	□	■	■	■	□	■
Proj 17	□	■	■	□	□	□
Proj 19	□	□	□	■	■	■
Proj 07	■	■	■	■	■	■
Proj 03	■	■	■	■	□	■
Proj 10	□	■	■	■	■	■
Proj 16	■	□	□	■	□	■
Proj 02	■	■	■	□	■	□
Proj 11	■	■	■	□	■	■

Fig. 21

Company	Disease 1	Disease 2	Disease 3	Disease 4	Disease 5	Disease 6	Disease 7	Disease 8	Disease 9	Disease 10	Disease 11	Disease 12
Company 1	Phase I		Phase II		LO/DE			LO/DE	Phase I		Phase II	Phase I
Company 2	Phase I	LI	Phase II			LI/LO	LI/LO	LI/LO	LI/LO	LI/LO		
Company 3	LI/LO				LI/LO	[illegible]	LI/LO		[illegible]	[illegible]		
Company 4	LO				LO/PL	Phase II	LO	Phase II			LO	
Company 5	LI/LO			LO	LO	Phase I	LO/DE			LO		TS/LI
Company 6	LO		[illegible]	[illegible]				[illegible]				
Company 7	LI/LO							Phase I	LO/DE	LI/LO	Phase I	LI
Company 8	LO/DE	Phase II			LO				LO		LO	
Company 9	LI/LO					Phase I	LI/LO	LI/LO	LI/LO		LI/LO	LI/LO
Company 10		LO		LO	Phase III					Phase II		
Company 11	LO			LO	LO							
Company 12	LO		Phase II		LO							LI/LO
Company 13	LI				Phase III		Phase III					LI
Company 14	LI/LO		LI/LO		LI/LO			LI/LO			LI/LO	
Company 15	LI		LI	LI	LI					LI		
Company 16	LI		LI		LI		Phase II					
Company 17	Phase II				LI/LO	LI/LO						
Company 18			Phase II					Phase I				
Company 19	LI		LI				LI					
Company 20				LI/LO								
Company 21	LI/LO				PhaseI/II							
Company 22	TS		TS			TS				TS		
Company 23	LI				LO/DE							
Company 24	LI											
Company 25	LI/LO											

Fig. 22

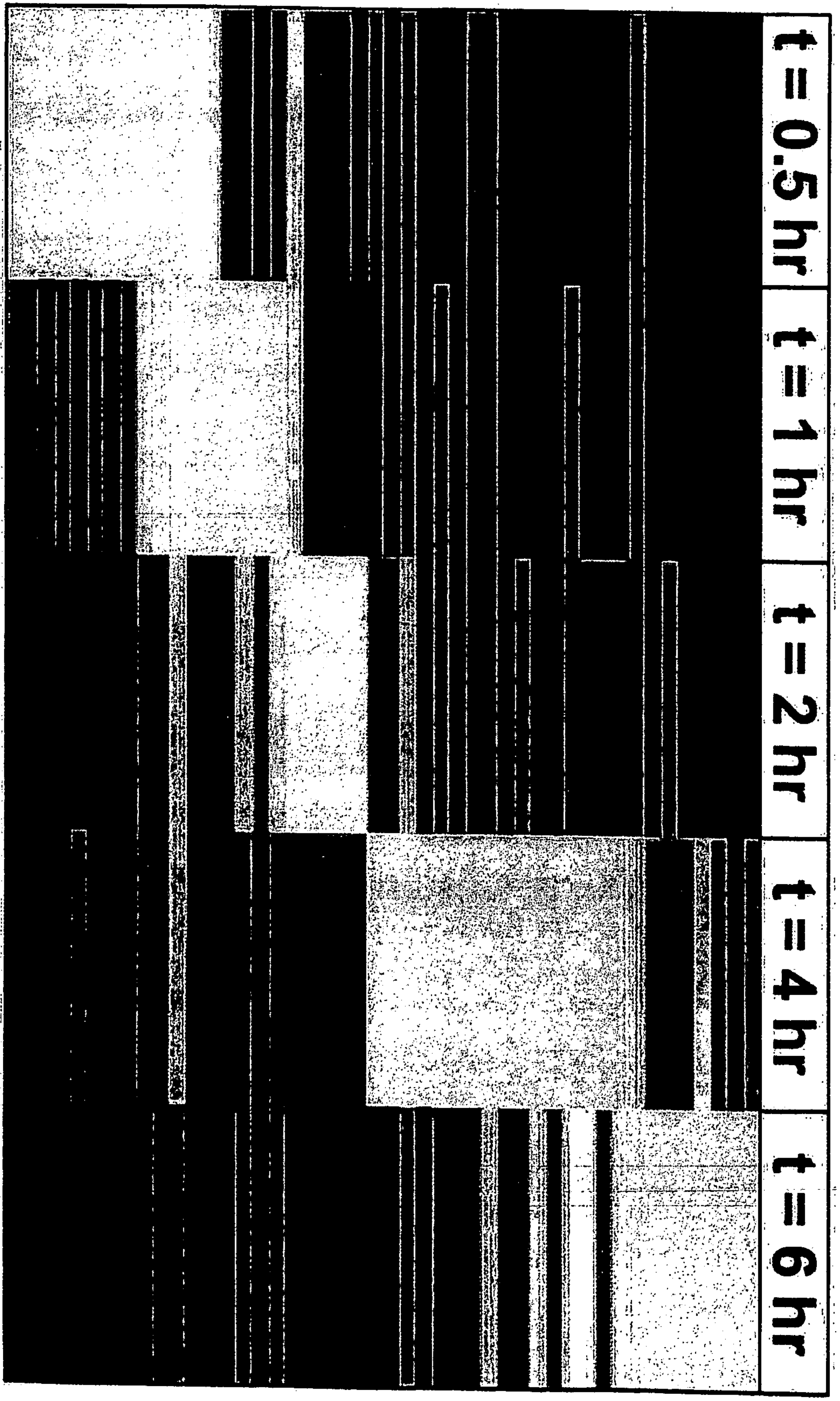


Fig. 23

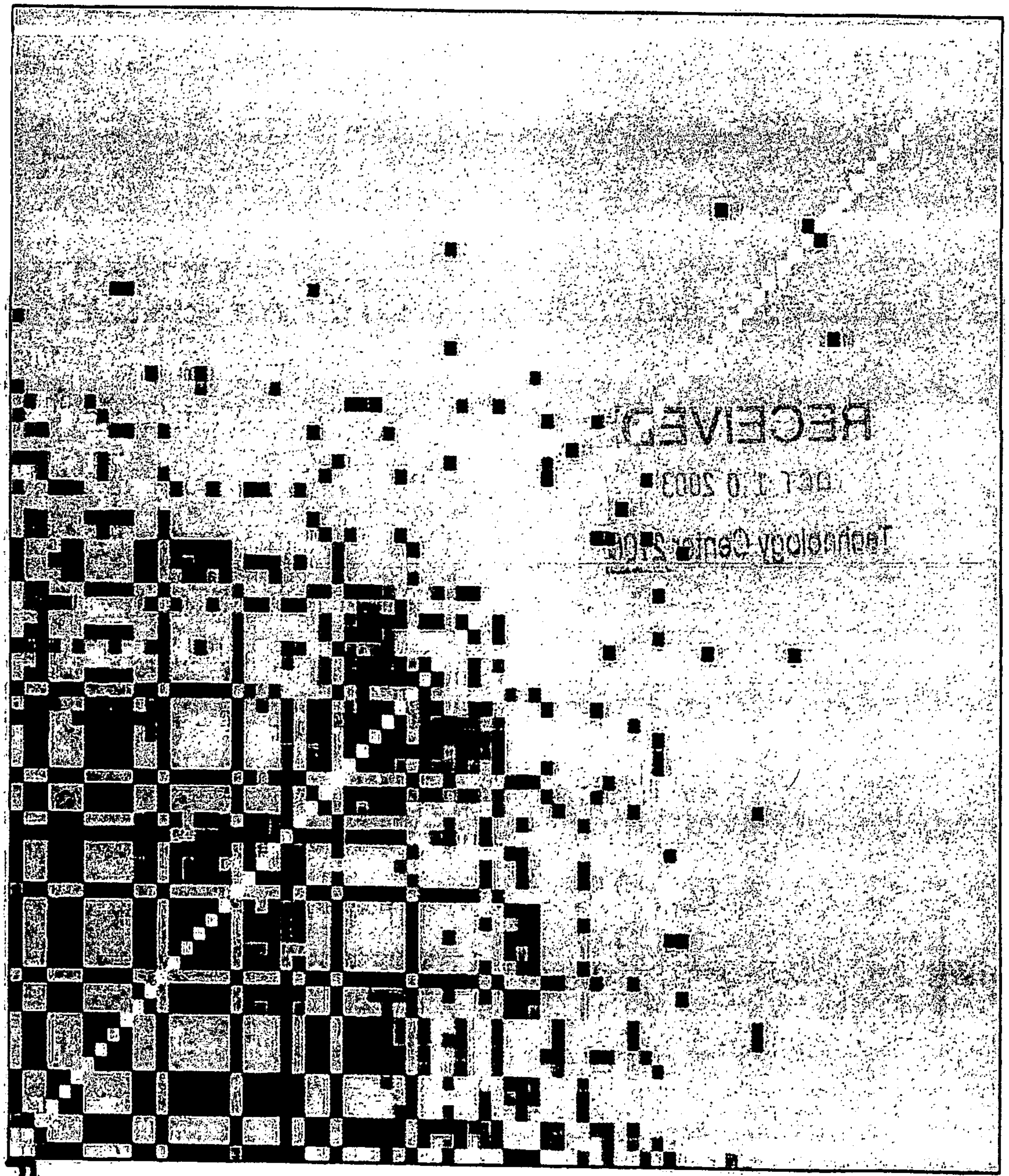


Fig. 24

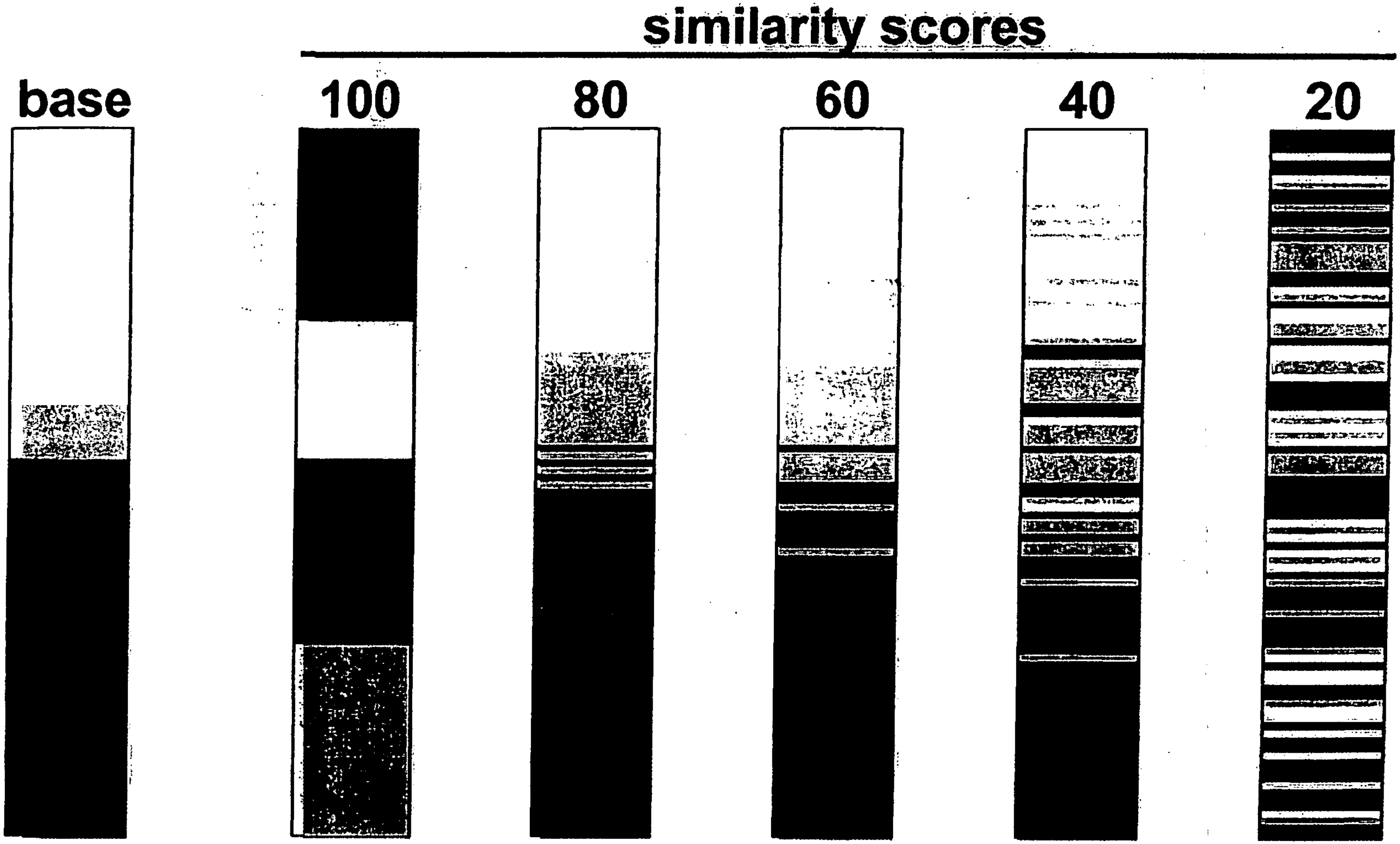
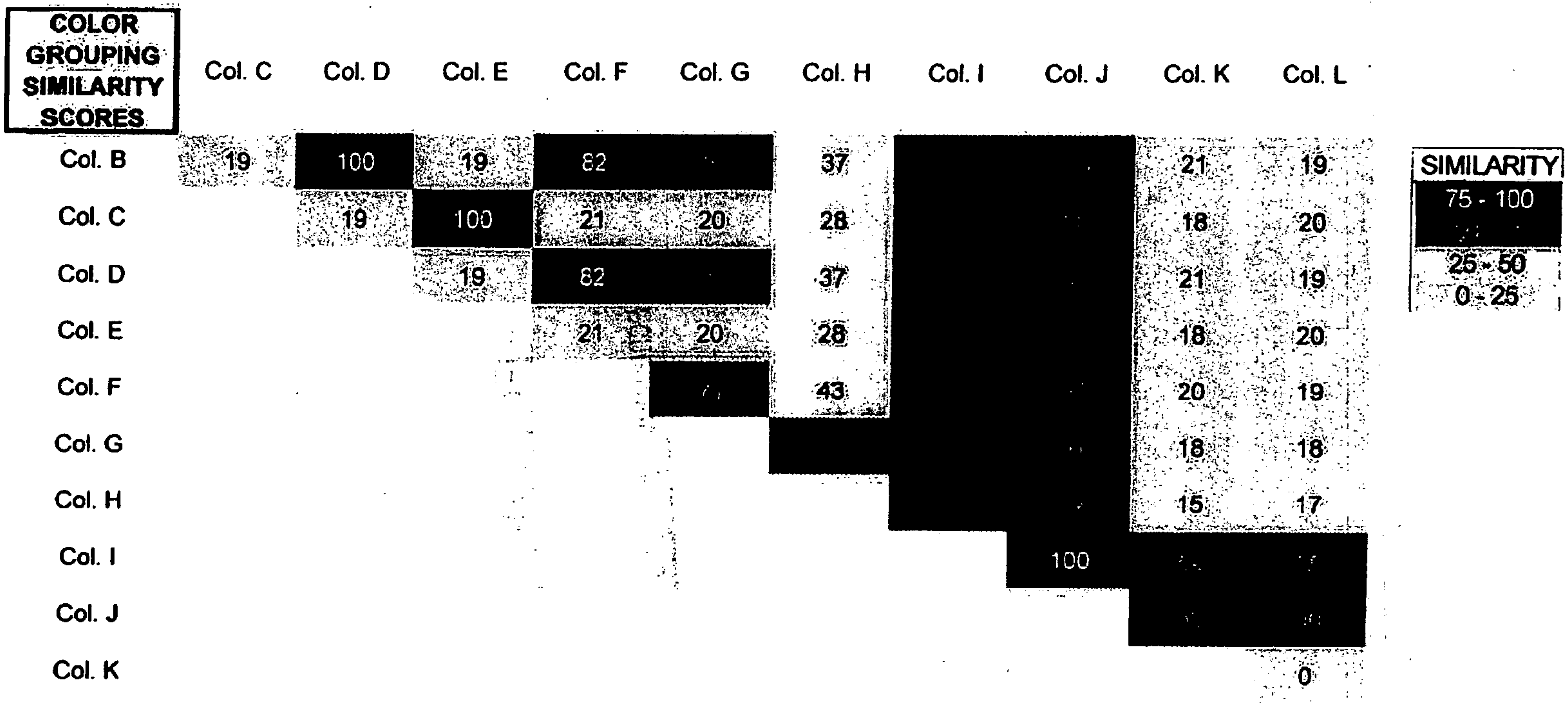


Fig. 25



COLOR GROUPING SIMILARITY SCORES	Col. C	Col. D	Col. E	Col. F	Col. G	Col. H	Col. I	Col. J	Col. K	Col. L
Col. B	19	100	19	82	[illegible]	37	[illegible]	[illegible]	21	19
Col. C		19	100	21	20	28	[illegible]	[illegible]	18	20
Col. D			19	82	[illegible]	37	[illegible]	[illegible]	21	19
Col. E				21	20	28	[illegible]	[illegible]	18	20
Col. F					[illegible]	43	[illegible]	[illegible]	20	19
Col. G						[illegible]	[illegible]	[illegible]	18	18
Col. H							[illegible]	[illegible]	15	17
Col. I								100	[illegible]	[illegible]
Col. J									[illegible]	[illegible]
Col. K										0

SIMILARITY
75 - 100
[illegible]
25 - 50
0 - 25

Fig. 26